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SCATTERING, REACTIONS and DECAY in NONRELATIVISTIC QUANTUM MECHANICS

Translated from Russian

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(Rasseyanie, reaktsii i raspady v nerelyativistskoi kvantovoi mekhanike)

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PREFACE

This monograph is intended mainly for postgraduate students and beginning theoretical physicists. Its aim is to fill the gap between standard text-books in quantum mechanics, on the one hand, and advanced-level books and periodical articles in the theory of quantized fields, on the other.

Traditional courses in quantum mechanics mostly deal with general principles and the theory of stationary states. Particular problems of scattering theory, unstable states, and multichannel processes are generally treated in greatly condensed form, so that the student cannot acquire sufficient knowledge and techniques for independent work in this field. On the other hand, noninitiates embarking on a course in the theory of quantized fields and the closely related relativistic quantum mechanics have to fight their way through a jungle of unfamiliar concepts associated with Lorentz invariance, causality, mass and charge renormalization, and introduction of particle creation processes.

In writing this book, we started with the premise that renormalization and creation problems can be studied in the nonrelativistic approximation, which is much more meaningful to the beginner.

The reader will find here a detailed treatment of the theory of scattering and the -matrix, will learn how to work with a continuum of states, and familiarize himself with the theory of unstable particles.

A substantial part of the book is based on the original researches of the authors. This includes the problem of scattering amplitude singularities when new channels are opened, the theory of unstable particles, the lifetime of intermediate states in scattering, a new formulation of the Lee model, nonrelativistic treatment of particle creation and nonconservation of parity.

The choice of material was thus of necessity somewhat subjective. We believe, however, that this shortcoming is at least partly compensated by the efforts all authors generally take over the presentation of their own results. We hope that the reader will find much interesting and useful information among the stimulating and complex problems which lie hidden in the depths of the commonplace, nonrelativistic quantum mechanics and in the familiar Schroedinger equation.

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Chapter 1

THE DISCRETE SPECTRUM

§ 1. INTRODUCTION

In this chapter we discuss some properties of the solutions of the Schroedinger equation which have a discrete spectrum of eigenvalues. These solutions, as we know, describe bound states. Three particular cases will be considered: (a) states with low binding energy, (b) bound states in a Coulomb field, (c) the states of a three-dimensional harmonic oscillator.

A bound state with energy ε small compared to the depth U_0 of the potential well is often encountered in applications; as an example, we can mention the ground state of a deuton. The properties of these states are treated in some detail in § 3, where particular stress is placed on the case $\varepsilon \to 0$, when the bound level has just formed. In § 4 we consider the motion of a particle in two or several potential wells and the important concept of a pseudopotential is introduced.

Fairly detailed treatment of cases (b) and (c) can be found almost in any standard textbook on quantum mechanics, and we will therefore concentrate only on the specific qualitative properties of these states. Here we have an example of degeneracy (generally called "accidental" degeneracy) of states with different values of the angular momentum l. Superpositions with various l values thus also constitute stationary states, and an alternative classification of levels can be developed in this case.

The expression "accidental" degeneracy is by no means to be understood literally! The situation here is by no means accidental. It is a consequence of a special property of classical mechanical systems, the existence of closed trajectories or paths. In quantum mechanics, degeneracy is a consequence of the separation of variables in several coordinate systems. A more fundamental reason, however, is the existence of a transformation group which leaves the Schroedinger equation invariant. All the other properties follow from the existence of this invariant group. These topics are discussed in § 5 for a Coulomb potential and in § 6 for the harmonic oscillator. The so-called "coherent" states are also discussed in § 6. These states, though not stationary, have a number of remarkable properties, e.g., they are the closest (in a certain sense of this word) to the properties of a classical oscillator.

Finally, § 7 gives a derivation of the so-called virial theorem and some of its generalizations are considered.

A few words of guidance to the reader.

The only purpose of § 1 and § 2 is to introduce the notation for future use. A reader who has recently taken a standard course in quantum mechanics is urged to stop here and to skip the rest of § 1 and all of § 2. Otherwise he may become prejudiced and put the book aside before even reaching those topics which are still unfamiliar to him and are of the main interest.

We will now briefly outline the fundamental postulates of quantum mechanics.

The state of a system in a nonrelativistic quantum mechanics is completely described by a wave function Ψ, whose variation in time is determined by the Schroedinger equation (henceforth abbreviated to Sch. Eq.)

$$i\hbar \frac{\partial \Psi}{\partial t} = H\Psi, \tag{1.1}$$

where H is the system Hamiltonian.

We will mainly consider the case when the Hamiltonian does not depend explicitly on time. In this case stationary states exists, for which the probability density $|\Psi|^2$ is constant in time. The wave function of a stationary state has the form

$$\Psi(t) = \psi e^{-\frac{iEt}{\hbar}};$$

whence it follows that ψ is an eigenfunction of the Hamiltonian,

$$H\psi = E\psi, \tag{1.2}$$

which describes a state with a certain real energy E.

For the case of a single particle in a constant external field we have

$$\left.\begin{aligned} H &= -\frac{\hbar^2}{2m}\Delta + U(r), \\ \left(-\frac{\hbar^2}{2m}\Delta + U(r)\right)\psi(r) &= E\psi(r). \end{aligned}\right\} \tag{1.2'}$$

The wave function $\psi(r)$ should satisfy the usual conditions: the function and its first derivative are single-valued* and continuous in the entire space.

In the applications the potential $U(r)$ is often spherically symmetric, i.e., it is a function of r only. In a spherically symmetric field the angular momentum operator $\boldsymbol{L}$ commutes with the Hamiltonian operator H (this corresponds to the conservation of angular momentum in classical mechanics). Moreover, the operator H commutes with the inversion operator P (this property is without analog in classical mechanics /7/).

Since the operators H, L^2, L_z, and P commute, the eigenvalues of H may simultaneously be the eigenvalues of L^2, L_z, and P. In other words, a stationary state may have a definite orbital momentum l, where $L^2 = l(l+1)$, l is an integer, a definite value of the momentum projection m on any axis z,

* The condition of single-valuedness of the wave function is treated in detail by Pauli /1, 2/. This condition leads, e. g., to such nontrivial effects as magnetic flux quantization in a multiply connected superconductor /3, 4/ and formation of quantized vortex "threads" in liquid helium /5, 6/.

m taking $(2l+1)$ values from $-l$ to $+l$, and a definite parity $P=+1$ or $P=-1$. In the one-particle problem the parity is uniquely fixed by the orbital momentum, $P=(-1)^l$, i.e., the parity of the state is equal to the parity of the number l.

It follows from the preceding that the Sch. Eq. has solutions of the form

$$\psi(r) = R_l(r)\, Y_{lm}(\theta, \varphi). \tag{1.3}$$

Here θ and φ are the polar and the azimuthal angle of the vector r, $Y_{lm}(\theta, \varphi)$ are the spherical functions, and $R_l(r)$ is a function which depends on r only. Insertion of (1.3) in (1.2) gives the following equation for R_l:

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR_l}{dr}\right) + \left[\frac{2m}{\hbar^2}(E-U) - \frac{l(l+1)}{r^2}\right]R_l = 0. \tag{1.4}$$

We introduce a new function

$$\chi_l(r) = rR_l(r), \tag{1.3'}$$

and the first derivative drops out from the Sch. Eq.

$$\chi_l'' + \left[k^2 - \left(V(r) + \frac{l(l+1)}{r^2}\right)\right]\chi_l = 0, \tag{1.5}$$

Here $k = \sqrt{2mE/\hbar^2}$ and $V = \frac{2m}{\hbar^2}U$. We will refer to V as the potential, whenever this need not cause confusion.

The centrifugal potential $\frac{l(l+1)}{r^2}$ can be incorporated in V, so that equation (1.5) takes the form

$$\chi_k'' + (k^2 - V(r))\chi_k = 0. \tag{1.6}$$

The properties of this equation are analyzed in any standard text on quantum mechanics (excellent treatment will naturally be found in Landau and Lifshitz's "Quantum Mechanics" /8/).

As $\psi(r)$ is bounded, we have the following boundary conditions for χ_k:

$$\left.\begin{aligned} &\chi_k(r) \to 0 \quad \text{for } r \to 0, \\ &\frac{\chi_k(r)}{r} \text{ bounded for } r \neq 0 \text{ and } r \to \infty. \end{aligned}\right\} \tag{1.7}$$

Moreover, χ_k and χ_k' should naturally be continuous. *

We further choose the point of zero energy in such a way that $V(r)$ vanishes for $r \to \infty$.

Almost all the interactions between particles that we find in nature (except the Coulomb force and a few other interactions) are described by rapidly decreasing potentials, i.e., potentials which fall off faster than $1/r$ for large r. In many cases these interactions are actually ignorable for all r greater than some R, so that we may take $V(r) = 0$ for $r > R$. We

* This is associated with the fact that equation (1.6) contains second derivatives: if either χ_k' or χ_k is discontinuous, the right-hand side of (1.6) will contain a δ- or a δ'-function, and no longer be equal to zero.

will thus speak of short-range potentials. Introduction of the cutoff radius R greatly simplifies the mathematics, and we start the discussion with the particular case of a short-range potential. The centrifugal potential may be treated as a short-range potential and, so as to avoid further complications, we take the orbital momentum l equal to zero.

We can now formulate our problem as follows:

Find all the solutions $\chi_k(r)$ of the equation

$$\left.\begin{aligned} \chi_k'' + (k^2 - V(r))\chi_k = 0 \quad &\text{for } r < R, \\ \chi_k'' + k^2\chi_k = 0 \quad &\text{for } r \geqslant R, \end{aligned}\right\} \tag{1.6'}$$

which satisfy conditions (1.7).

The wave function in this case is

$$\psi(r) = R_{k0}(r)\, Y_{00}(\theta, \varphi) = \frac{1}{\sqrt{4\pi}} \frac{\chi_k(r)}{r}. \tag{1.3''}$$

For $r > R$, as we see from the second equation in (1.6'), we have two solutions*

$$\chi_k^{(\pm)} = e^{\pm ikr}. \tag{1.8}$$

For $r < R$ we also have two solutions, but only one of them is acceptable, as the other does not satisfy the boundary conditions at $r = 0$. Indeed, χ_k for $r \to 0$ is sought in the form of a power function r^σ; then by (1.6')

$$\sigma(\sigma - 1) = -r^2(k^2 - V(r)).$$

If $r^2 V(r) \to 0$, we find two values for σ, namely 0 and 1. For $r \to 0$ the Sch. Eq. thus has two solutions

$$\psi_1(r) \to a \text{ for } r \to 0, \quad \psi_2(r) \to \frac{b}{r} \text{ for } r \to 0,$$

where a and b are constants. The solution ψ_2 must be rejected since

$$\Delta \frac{b}{r} = -4\pi b \delta(r)$$

so that for $r = 0$, ψ_2 does not satisfy the Sch. Eq.** We are left with the only solution ψ_1, which corresponds to the power index $\sigma = 1$.

The above treatment can be regarded as substantiating the boundary condition $\chi(r) \to 0$ for $r \to 0$. The solution which satisfies this boundary condition will be designated $\chi_k^{(0)}(r)$.

* In the case of rapidly falling potentials we also have two solutions $\chi_k^{(\pm)}(r)$ which behave as $e^{\pm ikr}$ for large r. These solutions are often written in symbolic form as $f(\mp k, r)$. Their properties were treated in some detail by Jost /9/, and in this way they earned the name of Jost functions. For potentials with a Coulomb tail, $U = \frac{\alpha}{r}$, the asymptotic behavior of the functions $\chi_k^{\pm}(r)$ for $r \to \infty$ is of the form $e^{\pm i(kr - \eta \ln 2kr)}$, where $\eta = \frac{m\alpha}{\hbar^2 k}$.

** A solution of this kind is used in case of a singular potential.

Now consider the regions of positive and negative energies.* Positive energies correspond to real values of k. In this case, the two solutions (1.8) remain bounded for all $r \geqslant R$, i.e., both solutions are acceptable in this region.

The most general solution for $r > R$ can be written in the form

$$\chi_k(r) = A(k)(\chi_k^{(-)} - S(k)\chi_k^{(+)}). \tag{1.9}$$

For $r = R$ this solution should match continuously the solution for the interior region:

$$\left.\begin{aligned} A(k)(\chi_k^{(-)} - S(k)\chi_k^{(+)})|_{r=R} &= \chi_k^{(0)}(R), \\ A(k)(\chi_k^{(-)'} - S(k)\chi_k^{(+)'})|_{r=R} &= \chi_k^{(0)'}(R). \end{aligned}\right\} \tag{1.10}$$

The matching can be ensured by an appropriate choice of A and S. Indeed, approaching (1.10) as a system of simultaneous equations for A and S, we readily find

$$\left.\begin{aligned} S(k) &= \left.\frac{\chi_k^{(-)'}\chi_k^{(0)} - \chi_k^{(-)}\chi_k^{(0)'}}{\chi_k^{(+)'}\chi_k^{(0)} - \chi_k^{(+)}\chi_k^{(0)'}}\right|_{r=R}, \\ A(k) &= \left.\frac{\chi_k^{(+)'}\chi_k^{(0)} - \chi_k^{(+)}\chi_k^{(0)'}}{2ik}\right|_{r=R}. \end{aligned}\right\} \tag{1.11}$$

Thus, for each positive energy value, the Sch. Eq. has one and only one solution. The physical meaning of this unique solution will be discussed in what follows.

For negative energies, the position is essentially different. Negative E correspond to imaginary k, i.e., $k = i|k|$.**

The solution $\chi_k^{(-)} = e^{|k|r}$ exponentially diverges for $r \to \infty$ and thus does not meet the second condition in (1.7). The most general solution for $r > R$ thus has the form

$$A(k)\chi_k^{(+)}(r), \tag{1.12}$$

and the matching condition for the interior and the exterior functions is

$$\left.\frac{\chi_k^{(+)'}}{\chi_k^{(+)}}\right|_{r=R} = \left.\frac{\chi_k^{(0)'}}{\chi_k^{(0)}}\right|_{r=R} = -|k|. \tag{1.13}$$

This condition is in fact a transcendental equation for $|k|$ and it is satisfied only by certain discrete imaginary values $k = k_n$ (or, correspondingly, discrete negative energies E_n).

We see from (1.13) that this relation can be satisfied only if the logarithmic derivative of $\chi_k^{(0)}$ is negative. This, as will become clear from what follows, is possible only if $V(r)$ is negative in the main (i.e., a repulsion potential) and has a large absolute value. In this case, the functions of the discrete spectrum for $r > R$ have the form

$$\chi_{k_n}(r) = A(k_n)\chi_{k_n}^{(+)}(r) = A(k_n)e^{-|k_n|r},$$

* The case of positive energies is treated in more detail in Chapter 2.

** We follow the usual convention which places k in the upper halfplane. In principle, of course, nothing prevents us from considering the value of k in the lower halfplane, when $\chi^{(+)}$ and $\chi^{(-)}$ are interchanged.

i.e., they decay exponentially for large r.* For $r < R$ these functions are also bounded, and the integral

$$\int_0^\infty |\chi_{k_n}(r)|^2\, dr \tag{1.14}$$

converges. The function χ_{k_n} is generally normalized so that this integral is equal to unity. Since χ_{k_n} falls off exponentially for $r > R$, the solution represents a localized state of a particle in space. The solutions of this type correspond to the classical case of bounded motion of a particle with negative energy, and the corresponding states are the bound states of quantum mechanics.

Thus, for positive energies, the Sch. Eq. has a unique solution (satisfying the boundary conditions) for each positive value of E (i.e., for $k^2 > 0$) and for any l.

For negative energies and fixed l, the equation is solvable (if at all) only for some discrete values $E = E_{nl}$. This result is generally formulated as follows: for positive energies, the energy eigenvalues constitute a continuous spectrum, whereas for negative energies the spectrum is discrete.

In a discrete spectrum, each level in general has a definite value of l. Levels with equal l and different m are degenerate, this being a consequence of the spherical symmetry of the potential.

However, for $l \neq 0$, the solutions themselves are not spherically symmetric; their angular dependence is determined by the angular part of the wave function, $Y_{lm}(\theta, \varphi)$.**

The solution moreover has a definite parity P. The degeneracy corresponding to different m for one l does not alter the situation: all the degenerate levels and any linear combination of these levels (which is also a solution) have the same parity P. The probability density $|\psi|^2$ (for a charged particle this is the charge density) is not affected by space inversion, since this transformation changes ψ either to ψ or to $-\psi$.

This proves that the charge density in a spherically symmetric potential always has a center of symmetry (although it need not be spherically symmetric), so that the electric dipole moment is always zero.

In the special case of a Coulomb potential $U = -\frac{Ze^2}{r}$ we encounter the so-called accidental degeneracy, i.e., levels with different l have exactly equal energies. The conclusion of zero dipole moment thus breaks down, and the particle may occupy a state with a finite dipole moment (this effect is treated separately in § 5).

* Note that for rapidly decreasing potentials the asymptotic behavior of $\chi_{k_n}(r)$ is described by $e^{-|k_n|r}$ for $r \to \infty$, whereas for potentials with a Coulomb tail $U(r) \sim \frac{\alpha}{r}$ for $r \to \infty$

$$\chi_{k_n}(r) \sim r^{-\eta_n} e^{-|k_n|r}, \quad \eta_n = \frac{m\alpha}{\hbar^2 |k_n|}.$$

** Note that the sum $\sum_{m=-l}^{l} |Y_{lm}(\theta, \varphi)|^2$ is independent of the angles θ and φ. Hence it follows that if for a given l the particle may occur with the same probability in all states with different m, the probability density of finding the particle at a certain point in space is spherically symmetric.
This explains, among other things, why the charge density in closed electron shells of an atom or in the closed shells of a nucleus is spherically symmetric.

§ 2. THE QUALITATIVE FORM OF THE WAVE FUNCTION

Consider the qualitative form of the solutions $\chi(r)$ of the Sch. Eq. We will discuss separately the regions with $k^2 < V(r)$ and $k^2 > V(r)$.

For $k^2 < V(r)$ the total energy is less than the potential energy and for $k^2 > V(r)$ the total energy is greater than the potential energy. The kinetic energy is thus respectively negative or positive.

The behavior of $\chi_k(r)$ will be examined in the quasiclassical approximation, * which is sufficiently faithful for purposes of qualitative treatment.

We write (1.6) in the form

$$\chi_k'' + \left(\frac{p}{\hbar}\right)^2 \chi_k = 0, \tag{1.6''}$$

where p is the classical momentum of the particle:

$$p(r) = \hbar \sqrt{k^2 - V(r)}.$$

The solution of (1.6'') is sought in the form

$$\chi(r) = e^{i\sigma(r)}. \tag{2.1}$$

For $\sigma(r)$ we thus obtain an equation

$$i\sigma'' - (\sigma')^2 + p^2/\hbar^2 = 0.$$

If (as is usually assumed) $\sigma'' \ll (\sigma')^2$, this equation yields

$$\sigma' = \pm \frac{p(r)}{\hbar}, \quad \sigma = \pm \frac{1}{\hbar} \int p(r')\, dr', \tag{2.2}$$

* In quantum mechanics this approximation was first introduced by Wentzel /10/. Kramers /11/, and Brillouin /12/, and it is correspondingly designated as the WKB approximation. The quasiclassical approximation received the main impetus in connection with the solution of quantum-mechanical problems, although Liouville /13/ and Rayleigh /14/ already approached individual problems by a similar technique (on this subject see /15/, where an extensive bibliography will be found; this book also gives solutions of various particular problems). A different approach is given in /16/. Notice that the quasiclassical approximation was developed in maximum detail for the one-dimensional Sch. Eq. with a time-independent potential. An example of a quasiclassical solution for a time-dependent potential will be found in /17/. For many-dimensional problems a useful technique is generally to change over to new coordinates in which the variables in the Sch. Eq. can be separated, so that the problem is reduced to the one-dimensional case. In the three-dimensional case of free motion, say, the variables are separable in ten coordinate systems besides the spherical system /18/. If one fails to find a coordinate system with separable variables, the derivation of the quasiclassical solution is a difficult problem. An example of this kind for the two-dimensional case is examined in /19/. In /236/ it is also shown that in a number of cases quantum-mechanical approach sheds new light on the results of classical mechanics.

whence

$$\chi = \exp\left\{\pm \frac{i}{\hbar}\int p(r')\,dr'\right\}. \tag{2.3}$$

The condition of applicability of this method is clearly the following:

$$\left|\frac{\sigma''}{(\sigma')^2}\right| = \left|\frac{p'\hbar}{p^2}\right| = \left|\frac{d\lambda(r)}{dr}\right| \ll 1. \tag{2.4}$$

Here λ is the de Broglie wavelength of the particle $\left(\lambda(r) = \frac{\hbar}{p(r)}\right)$. This condition is satisfied only for sufficiently smooth potentials, far from the points where $p(r)$ is zero (the turning points). For real potentials, condition (2.4) holds true in a wide range of r values.

In the classically accessible region $k^2 > V(r)$ (i.e., $E > U(r)$), the two independent solutions may be written in the form

$$\begin{matrix}\sin \\ \cos\end{matrix}\left\{\frac{1}{\hbar}\int_{r_0}^{r} p(r')\,dr'\right\}, \tag{2.5}$$

i.e., both solutions are oscillating functions. The frequency of these oscillations increases as the difference $(k^2 - V(r)$ becomes greater.

The case $k^2 < V(r)$ corresponds to a classically inaccessible region, where $E < U(r)$. Here, p takes on imaginary values $p = i|p|$ and the two independent solutions are the monotonic functions

$$\chi_1 = e^{\frac{1}{\hbar}\int_{r_0}^{r}|p(r')|dr'}, \quad \chi_2 = e^{-\frac{1}{\hbar}\int_{r_0}^{r}|p(r')|dr'} \tag{2.6}$$

To summarize:

In the classical region, the Sch. Eq. has two oscillating solutions. The frequency of oscillations increases with increasing difference $k^2 - V(r)$.

In the nonclassical region, the Sch. Eq. also has two solutions, but they are both monotonic. One of these solutions decreases from the point where $k^2 = V(r)$ and the other increases.

§ 3. LOW-ENERGY BOUND STATES

Consider the Sch. Eq. with $U(r) < 0$. Note that in this case the fundamental distinction between classical and quantum mechanics can be formulated as follows. In classical mechanics any arbitrarily small potential well is sufficient to bind the particle; the particle will rest at the bottom of the well, which corresponds to a solution with $E = U_{\min} < 0$.

In quantum mechanics, in the three-dimensional case, we are dealing with certain critical conditions for the existence of at least one discrete level; for such a level to exist, the well should be sufficiently "wide and deep". This result is clearly traceable to the uncertainty principle: a particle is bound by the potential $U(r)$ if it remains a certain proportion of the time in a region where the potential is negative, but not zero. The localization of the particle in space, however, implies an increase in its mean momentum

and mean kinetic energy. Therefore in a shallow and narrow well it is impossible to construct a solution with negative total energy, and not a single discrete level can be accommodated. *

Of considerable importance are the conditions which prevail when a discrete level has just formed, i.e., when the depth and the width of the well are close to their critical values. A characteristic feature of the solution in this case is that the particle remains a very short time in the well (this time goes to zero as the well approaches its critical dimensions), and the properties of the solution are not oversensitive to the form of $U(r)$. A situation of this kind is encountered, say, in the theory of the deuton, which is a bound proton—neutron state /21/.

Let us first derive the condition for the existence of a discrete level in a "rectangular well", i.e., in a potential of the form

$$\left.\begin{aligned} U = -U_0 = -\tfrac{\hbar^2}{2m}V_0 \quad & \text{for } r \leqslant R, \\ U = 0 \quad & \text{for } r > R. \end{aligned}\right\} \tag{3.1}$$

The Schroedinger equation (1.6) takes the form

$$\left.\begin{aligned} \chi'' + (-\varkappa^2 + V_0)\chi = 0 \quad & \text{for } r \leqslant R, \\ \chi'' - \varkappa^2\chi = 0 \quad & \text{for } r > R. \end{aligned}\right\} \tag{3.2}$$

Here we use the notation $\varkappa = -ik$. Since we are concerned with bound states, whose energy is negative, k is a pure imaginary number ($k = i|k|$), so that $\varkappa$ is real, $\varkappa = |k|$.

The solutions of (3.2) satisfying the boundary conditions are

$$\left.\begin{aligned} \chi = B\sin Kr, \quad K = \sqrt{V_0 - \varkappa^2} \quad & \text{for } r \leqslant R \\ \chi = Ae^{-\varkappa r} \quad & \text{for } r > R. \end{aligned}\right\} \tag{3.3}$$

Equating these functions and their derivatives at the matching point $r = R$, we find

$$\left.\begin{aligned} B\sin KR = Ae^{-\varkappa R}, \\ BK\cos KR = -\varkappa Ae^{-\varkappa R}. \end{aligned}\right\} \tag{3.4}$$

We can now determine the potential $-U = U_1$ required for the formation of a bound state. The energy of a state which has just formed is clearly zero. Therefore putting $\varkappa = 0$ in (3.4) we obtain

$$\sqrt{V_1}R = \frac{\pi}{2}; \quad V_1 = \frac{\pi^2}{4}\frac{1}{R^2}; \quad U_1 = +\frac{\pi^2\hbar^2}{8mR^2}.$$

The dependence $U_1 \sim R^{-2}$ is quite general, and is not specific of a rectangular well only. Indeed, suppose that for some $U(r)$ the Sch. Eq. has a solution $\psi(r)$ with a given energy E. Try a substitution $\psi(r) \to \psi_1(r) = \alpha^{3/4}\psi(\alpha r)$. The factor $\alpha^{3/4}$ before ψ is so chosen that the wave function remains normalized; as the Sch. Eq. is linear, this factor cancels out.

* This argument is not quite conclusive, as in principle it is applicable also to the one-dimensional and two-dimensional case, when a discrete level exists irrespective of the well depth and width. Also note that any shallow well will acquire a discrete level as soon as an arbitrarily weak magnetic field is turned on /20/.

To identically satisfy the Sch. Eq. with the new ψ, we should make the substitution $E \to E_1 = \alpha^2 E$ and $U(r) \to \alpha^2 U(\alpha r)$, since

$$\frac{\hbar^2}{2m}\Delta_r\psi(\alpha r) + \alpha^2(-U(\alpha r) + E)\psi(\alpha r) = \alpha^2\left[\frac{\hbar^2}{2m}\Delta_{\alpha r} - U(\alpha r) + E\right]\psi(\alpha r) \equiv 0.$$

Thus, a contraction transformation ($\alpha > 1$, the characteristic length is α^{-1}) is accompanied by an increase in all energies by a factor $\sim\alpha^2$, i.e., in inverse proportion to the square of the linear dimensions. The physical reason for this is that the momentum is inversely proportional to wavelength, so that the kinetic energy is inversely proportional to the wavelength squared.

Consider the case $|\varkappa^2| \ll V_0$. We will calculate the probabilities w_1 and w_2 for the particle to be found inside the well ($r < R$) or outside the well ($r > R$), respectively. These probabilities are proportional to $w_1 \sim \int_0^R \chi^2\,dr$ and $w_2 \sim \int_R^\infty \chi^2\,dr$, and their sum is $w_1 + w_2 = 1$ by normalization condition.

Ignoring $\varkappa^2$ compared to V_0 in the radicand in (3.3) and taking $\sqrt{V_0}R \approx \frac{\pi}{2}$, we find

$$\frac{w_1}{w_2} = \frac{\pi}{2}\sqrt{\frac{\varkappa^2}{V_0}}. \tag{3.5}$$

Thus for $\frac{\varkappa^2}{V_0} \to 0$ the particle remains most of the time outside the well.

The mean potential energy is

$$\bar{U} = \int U|\psi|^2\,dr \approx -\frac{\pi}{2}\frac{\hbar^2}{2m}\sqrt{V_0\varkappa^2} = -w_1U_0.$$

The expectation value of the kinetic energy is

$$\bar{T} = \frac{\hbar^2}{2m}\int|\nabla\psi|^2\,dr \approx \frac{\pi}{2}\frac{\hbar^2}{2m}\sqrt{V_0\varkappa^2} = +w_1U_0.$$

Since $|\bar{U}| \gg |E|$, $\bar{T} \gg |E|$, the binding energy $\varepsilon = -E = -(\bar{U} + \bar{T})$ is a small difference between two large numbers. In order to find E as a sum $\bar{U} + \bar{T}$, we should compute the higher terms in the expansion of $\bar{U}$ and $\bar{T}$ in powers of $\varkappa^2/V_0$, which is left to the reader.*

For a given R there is a certain critical U_1 such that $E = 0$. Let us now gradually make the potential well "deeper" and see how the binding energy changes.

Using the perturbation theory, we find

$$dE = w_1\,dU \approx \frac{\pi}{2}\sqrt{\frac{|E|}{U_1}}\,dU.$$

* It is readily seen that in the one-dimensional case, for

$$\varkappa^2/V_0 \to 0,\ w_1/w_2 \approx \varkappa^2/V_0 = 4V_0R^2,\ \bar{U} \approx -\hbar^2\varkappa^2/2m,$$

we have $\bar{T} \approx \frac{1}{12}\frac{\varkappa^2}{V_0}|\bar{U}|$, i.e., $\bar{T} \ll |\bar{U}|$, so that there is always a level with energy $E \approx \bar{U} = -\frac{\hbar^2}{2m}4V_0^2R^2$. In the two-dimensional case a bound level also always exists, but the binding energy cannot be found in this way, since then $\bar{T} \approx |\bar{U}|$ and $E = \bar{T} - |\bar{U}|$ is an exponentially small number.

Hence

$$-2d\sqrt{-E} = \frac{\pi}{2}\frac{dU}{\sqrt{U_1}}, \quad \varepsilon = -E = \frac{\pi^2}{16}\frac{(|U|-U_1)^2}{U_1}. \tag{3.6}$$

The binding energy as a function of well depth thus has a characteristic singularity: at the point where the level forms, it is tangent to the abscissa axis (Figure 1). This is a general conclusion independent of the particular form of the potential $U(r)$.

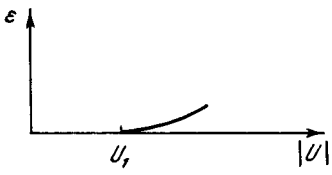

FIGURE 1.

Let us now consider a particle which occupies a bound level with $E = -|E_0|$ or scattered particles with energy of the order of $|E_0|$. The well depth is assumed to be large compared to $|E_0|$. In the limiting case as $E_0/U \to 0$ the theory is essentially simplified. Here for a fixed E_0 we make $|U|$ go to infinity; moreover $R \to 0$ in such a way that $|U|R^2 \to$ const.

The particular situation which develops during the formation of a level thus settles the question of the properties of the solution for a singular potential with $|U| \to \infty$ and $R \to 0$ for fixed binding energy.

The solutions of the Sch. Eq. and their derivatives should remain continuous for $r = R$:

$$\psi_1 = \psi_2, \quad \frac{d\psi_1}{dr} = \frac{d\psi_2}{dr}.$$

These two conditions can be rewritten in the form

$$\psi_1 = \psi_2, \quad \frac{1}{\psi_1}\frac{d\psi_1}{dr} = \frac{1}{\psi_2}\frac{d\psi_2}{dr} \quad \text{for } r = R.$$

The first condition is trivial, since the equation is linear and any ψ_1 which does not meet the first condition can always be multiplied by a constant C such that $C\psi_1|_{r=R} = \psi_2|_{r=R}$. This will not affect $\frac{1}{\psi_1}\frac{d\psi_1}{dr}$, however, so that the second condition is not trivial.

By matching the solution inside the well with the solution outside the well $\psi_2 \sim \frac{e^{-\varkappa_0 r}}{r}$, we find for $r = R$ (and in the limit as $R \to 0$, for $r = 0$)

$$\frac{d\ln\chi}{dr} = -\varkappa_0. \tag{3.7}$$

It is significant that in the limit as $R \to 0$ interchanging E_0 and E (which involves a small change in energy compared to U_0) does not affect the wave function $r < R$, and thus does not change the boundary condition (3.7) either.

A deep potential well is thus described by the value of $\frac{d\ln\chi}{dr}$ at the well boundary, this being a general property of the Sch. Eq.

Consider as an example the solution of the Sch. Eq. for a continuous spectrum of positive energies (in more detail this case is treated in Chapter 2). In this case the continuum functions are changed by the

potential well and the particle is scattered. Outside the well the equation has the form

$$\chi'' + k^2\chi = 0.$$

The general solution is thus

$$\chi(r) = A \sin(kr + \delta(k)). \tag{3.8}$$

In the absence of a potential well, we should have $\chi(0) = 0$, so that $\delta = 0$.

For a particle impinging on a potential well, we match the solution (3.8) with the solution inside the well, which gives

$$\frac{d \ln \chi}{dr}\Big|_{r=0} = k \cot \delta = -\varkappa_0, \quad \delta = \tan^{-1}\left(-\frac{k}{\varkappa_0}\right). \tag{3.9}$$

The linearity of the Sch. Eq. is responsible, to use mathematical terminology, for the group property of the solutions: any solution can be multiplied by a constant and still remain a solution. Using this group property, we can lower the order of the Sch. Eq. and switch over to a first-order nonlinear equation. This equation is conveniently written using a new variable $z = \frac{d \ln \chi}{dr}$.

Note that

$$\frac{d\chi}{dr} = z\chi, \quad \frac{d^2\chi}{dr^2} = \left(\frac{dz}{dr} + z^2\right)\chi$$

so that the Sch. Eq. is reduced to the form

$$\frac{dz}{dr} + z^2 - V(r) = -k^2, \tag{3.10}$$

The characteristic property of the regular solution with $\chi(0) = 0$, in which we are interested, is that for $r \to 0$, $\chi(r) \to Cr$ and $z \to \frac{1}{r}$. This transformation to a first-order equation is a general property of the Sch. Eq. *

The distinctive feature of the problem with a singular potential, i.e., a deep and narrow well, is that k^2 can be dropped inside the well, so that we have to solve the equation

$$\frac{dz}{dr} + z^2 - V(r) = 0 \tag{3.11}$$

and find z at the well boundary (i.e., $z(R)$), as it determines the solution outside the potential well. For $V \to \infty, R \to 0$ the inclusion of k^2 in the equation does not affect the result for $z(R)$.

As we have already noted, $V(r)$ should meet a certain precise condition if this deepening and narrowing of the potential well, i.e., the transformation

* In some cases this transformation is quite helpful. In particular, it sometimes facilitates the determination of scattering phases from the given potential $U(r)$ /22/.

$V \to V_1(r) = \alpha^2 V(\alpha r)$, is to leave the binding energy $-E$ (and thus $z(R)$) finite. This condition is not written in explicit form, and it is only formulated as a constraint on the solutions of the Sch. Eq. If this condition is not satisfied, then $|E| \to \infty$ and $z(R) \to \infty$ for $\alpha \to \infty$.

The parameter $a = -\frac{1}{z}\Big|_{r=R}$ is called the scattering length. *

We have seen that $z < 0$ whenever a bound state exists. The scattering length in this case is positive. If the scattering length is negative, there is no bound state.

The entire theory of this section is not restricted to the lowermost energy level: in principle we can think of a case when the lowermost level (the wave function χ_1) lies very deep, $E \sim U$, and it is the second level χ_2 which is a "resonance" level close to the free states. The corresponding wave functions are shown in Figure 2.

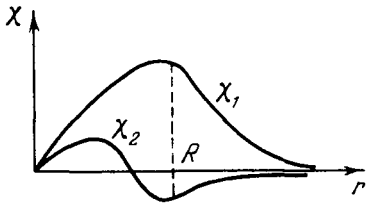

FIGURE 2.

In principle, resonances are also possible in a state with $l \neq 0$. In this case there is invariably a lower-lying level with $l = 0$. Note that for $l \neq 0$ the dependence of the scattering phase on E and the dependence of E on $(|U| - U_1)$ differs from that described by the above formulas for $l = 0$. We will not discuss this problem, however.

The two principal cases when the true potential $U(r)$ can be replaced with adequate accuracy by the limiting potential $U \to \infty$, $R \to 0$ are encountered in nuclear physics. The interaction between a neutron and a proton with $l = 0$ produces a bound state (a deuton nucleus) with binding energy of 2.2 MeV if the spins of the particles are parallel. This state can be described by a potential well whose depth U_0 is about 36 MeV and radius $R = 2 \cdot 10^{-13}$ cm. The second case of proton–neutron interaction with antiparallel spins is characterized by $z > 0$. No bound state forms in this case. The parameter $\frac{\hbar^2 z^2}{2m}$, called the virtual level energy, is equal to 0.07 MeV. The corresponding well parameters are $U_0 \approx 18$ MeV, $R = 2.5 \cdot 10^{-13}$ cm. Thus, the theory of singular potential is perfectly applicable to scattering of neutrons with energies of up to 1 MeV by protons.

§ 4. A PARTICLE IN THE FIELD OF SEVERAL SINGULAR POTENTIALS

In the preceding section we saw that the problem of motion of a particle in the field of a singular potential can be formulated in the language of boundary conditions imposed on the wave function at $r \approx 0$. The general solution of the Sch. Eq. for small r and $l = 0$ has the well-known form

$$\psi = \alpha + \frac{\beta}{r}, \quad \chi = r\psi = \alpha r + \beta. \tag{4.1}$$

* This concept was first introduced by Fermi /23/.

If we are dealing with smooth potentials, the constant β is taken equal to zero. This is not so, however, for a singular potential, and the boundary condition establishes a certain relation between the constants α and β:

$$\frac{1}{\chi}\frac{d\chi}{dr}\Big|_{r=0} = \frac{\alpha}{\beta} = z, \tag{4.2}$$

where z is a characteristic of the potential.

This approach is highly convenient for solving problems with several potentials.

Consider, for example, the case of two potential wells with given z, situated at the points r_1 and r_2. For a given energy $E = -\frac{\hbar^2\varkappa^2}{2m}$, the solution is sought in the form

$$\psi = \frac{e^{-\varkappa|r-r_1|}}{|r-r_1|} + \frac{e^{-\varkappa|r-r_2|}}{|r-r_2|}\cdot * \tag{4.3}$$

Near $r = r_1$, putting $r_{12} = |r_1 - r_2|$ and series expanding the first exponential, we have

$$\psi = \frac{1}{|r-r_1|} - \varkappa + \frac{e^{-\varkappa r_{12}}}{r_{12}}\cdot \tag{4.4}$$

Hence,

$$z = \frac{e^{-\varkappa r_{12}}}{r_{12}} - \varkappa. \tag{4.5}$$

This transcendental equation for $\varkappa$ enables us to find the binding energy of a particle in the field of two potential wells. In particular, we see that for $z > 0$ (i.e., a well which alone cannot bind the particle) two sufficiently close wells will produce a bound state; the critical condition is $r_{12} = \frac{1}{z}$ for $\varkappa = 0$.

Now consider the case of an infinite number of wells distributed in space with a density of ρ wells per cubic centimeter.

By analogy with the case of two wells, we have

$$\psi = \sum_i \frac{e^{-\varkappa|r-r_i|}}{|r-r_i|}\cdot \tag{4.3'}$$

The parameter $\varkappa$ is found from the condition

$$z = -\varkappa + \sum_i \frac{e^{-\varkappa r_{1i}}}{r_{1i}}\cdot \tag{4.5'}$$

The sum is replaced by an integral assuming that $\frac{1}{\varkappa}$ is much greater than the distance to the nearest neighbor, $\frac{1}{\varkappa} \gg \rho^{-1/3}$:

$$z = -\varkappa + \rho\int\frac{e^{-\varkappa r}}{r}\,dr = -\varkappa + 4\pi\rho\frac{1}{\varkappa^2}\cdot \tag{4.6}$$

* A similar wave function was used in the problem of pion scattering by a deuton in the momentum approximation /24/, and in collision problems involving negative ions and neutral atoms /25, 26/.

This equation, unlike the preceding case of two wells, always has a solution with $\varkappa > 0$, for any ρ and z. Since $1/\varkappa \gg \rho^{-1/3}$ we can drop $\varkappa$ compared to $4\pi\rho/\varkappa^2$. This gives

$$\varkappa^2 = 4\pi\rho\frac{1}{z}; \quad E = -4\pi\rho\frac{1}{z}\frac{\hbar^2}{2m}, \tag{4.7}$$

and the constraint $1/\varkappa \gg \rho^{-1/3}$ now takes the form $\frac{1}{z} \ll \rho^{-1/3}$. The entire treatment corresponds to the case $z > 0$, when a single well does not have a bound level.

We see that a system of wells distributed with a given density gives rise to a negative energy state. This energy is the same as if each well were replaced by a slowly varying potential $\tilde{U}(r)$ (whose variation is slow compared to the distance between the wells) satisfying the condition

$$\int \tilde{U}(r)\,dr = -4\pi\frac{\hbar^2}{2m}\frac{1}{z}.$$

Then the potential at any point, $\sum_i \tilde{U}(r - r_i)$, is constant throughout the entire volume, being equal to

$$\tilde{U} = -4\pi\rho\frac{\hbar^2}{2m}\frac{1}{z}. \tag{4.8}$$

This is also the energy of a particle at rest in the field of this potential.

This is the method for finding the slowly varying pseudopotential* and the small potential (to which the perturbation theory is applicable) whose action on a particle is equivalent to that of a singular well.

We should stress that the pseudopotential $\tilde{U}$ cannot be found by simple averaging of the potential $U(r)$: $U_{av} = \rho \int\limits_{V=\frac{1}{\rho}} U dr$. Thus, in the case of an attractive potential ($U < 0$), the pseudopotential is greater than the average potential, $|\tilde{U}| > |U_{av}|$, this being due to the increased probability of finding the particle in the region where the potential is different from zero. This result emerges with particular clarity when $U \sim \frac{\text{const}}{R^2}$ for $R \to 0$. Then $U_{av} = \text{const}\ \rho R \to 0$, whereas the pseudopotential $\tilde{U}$ does not approach zero. In the case of a repulsive potential ($U > 0$), $|\tilde{U}| < |U_{av}|$ and in the limit $U \to \infty$, $R \to 0$, $z \to \frac{1}{R}$, $\tilde{U} \sim \text{const} \cdot R \to 0$, whereas for $U = \text{const} \cdot \frac{1}{R^N}$ and $N > 3$ the limiting value is

$$U_{av} = \text{const} \cdot \rho \frac{1}{R^{N-3}} \to \infty.$$

Using the concept of a pseudopotential, we can easily find the refractive index of matter.

* This concept was first introduced by Fermi /23/. The applicability of the perturbation theory is considered in detail in Bethe's paper /27/ (p. 123) and in /28/.

Let a particle with small but finite energy $E = \frac{\hbar^2}{2m}$ be incident from vacuum into a medium characterized by pseudopotential $\tilde{U}$ (see (4.8)). For the kinetic energy T of the particle inside the medium we have

$$T = E - \tilde{U} = \frac{\hbar^2 k^2}{2m}\left(1 + \frac{4\pi\rho}{k^2}\frac{1}{z}\right) = \frac{(\hbar k n)^2}{2m}.$$

Hence an expression for the refractive index of the material:

$$n^2 = 1 + \frac{4\pi\rho}{k^2}\frac{1}{z} = 1 - \frac{4\pi\rho}{k^2}a. \tag{4.9}$$

Note that a well without a bound level ($U > 0$, say) nevertheless produces effective attraction; the corresponding pseudopotential is always negative, and the parameter z for $U \to \infty$ and fixed R monotonically approaches $\frac{1}{R}$.

Conversely, a well in which a bound level has just formed may capture a particle on that level. The other free particles, however, see this well as a center of repulsion and its pseudopotential is positive. This is the reason, for example, for the reflection of low-energy neutrons off the surface of graphite and beryllium at any incidence angle, up to the case of normal incidence. This effect opens an interesting possibility for cold neutron storage in a graphite container /29/.

As the well is made deeper, while its radius remains constant, the parameter z drops to minus infinity, then increases to plus infinity and eventually decreases reaching zero at the time when the second level is formed. This indicates that a change in well depth causes oscillation of the pseudopotential.

§ 5. COULOMB POTENTIAL

The theory of a particle in a Coulomb field was developed in great detail and can be found in any textbook. The monograph by Bethe and Salpeter /30/, for example, contains a wealth of information on the subject and a summary of published results up to 1959 inclusive.

In this section our aim is therefore not to present new results, but to examine the well-known facts from a different angle.

In the nonrelativistic approximation, when the relativistic corrections, the electron spin, and the higher approximations of quantum electrodynamics are ignored, the Hamiltonian of an electron in the Coulomb field of a nucleus of charge Ze is

$$H = -\frac{\hbar^2}{2m}\Delta - \frac{Ze^2}{r}, \tag{5.1}$$

and the energy levels are given by

$$E_n = -\frac{Z^2 e^4 m}{2\hbar^2}\frac{1}{n^2} = -\frac{E_0}{2n^2}. \tag{5.2}$$

Here

$$E_0 = \frac{Z^2 e^4 m}{\hbar^2} = 27\, Z^2\, \text{eV}.$$

We know from the elementary theory that the levels of a hydrogen atom are degenerate: for a given n, there are levels with l ranging from 0 to $n-1$; all these levels with different l have the same energy. This is known as "accidental" degeneracy,* as no such degeneracy is expected in the general theory of an arbitrary spherically-symmetric potential.

What new effects are associated with the accidental degeneracy? One of the best known is the linear Stark effect in the hydrogen atom: the excited hydrogen atoms, i.e., atoms with $n > 1$, may have different energies in the electric field. These atoms form a multiplet, the energy splitting being proportional to the electric field $\mathscr{E}$:

$$E = -\frac{E_0}{2n^2} + ka\,|\mathscr{E}|, \tag{5.3}$$

where k goes from $-(n-1)$ to $(n-1)$. Thus, for instance, the level with $n = 2$ is split into three sublevels.

The linear dependence of E on $|\mathscr{E}|$ signifies that the excited hydrogen atoms have an electric dipole moment: the energy of a neutral body with dipole moment $\boldsymbol{d}$ in an electric field $\mathscr{E}$ is $-\boldsymbol{d}\mathscr{E}$.

In § 1 we have demonstrated in a general way that an atom has no dipole moment. What is happening here then? States with a definite l in a Coulomb potential have no dipole moment. But here on account of accidental degeneracy we have, say, $E_{20} = E_{21} = E_2$ (the first index is the principal quantum number, the second index is l). Therefore a superposition of solutions with different l and the same n is also a solution corresponding to a given E_n.

Consider the states

$$\frac{1}{\sqrt{2}}(\psi_{2,0,0} + \psi_{2,1,0}) \quad \text{and} \quad \frac{1}{\sqrt{2}}(\psi_{2,0,0} - \psi_{2,1,0})\ .** \tag{5.4}$$

These are states with energy E_2 and dipole moments of $+3ea$ and $-3ea$, respectively, pointing along the z axis. Finally, $\psi_{2,1,1}$ and $\psi_{2,1,-1}$, as well as any superposition (linear combination) of these functions, are two states with energy E_2 and zero dipole moment.

Thus, from the four degenerate states (one $2S$ and three $2P$) we may form without any electric field two states with a dipole moment and two states without a dipole moment, all having the same energy.

In an electric field the level with $n = 2$ is split into three levels.

States with dipole moment do not have a definite parity, since they are formed as superpositions of states of opposite parity.

* As distinct from the degeneracy of levels with fixed l and various m, which is a consequence of the invariance of the Sch. Eq. under three-dimensional rotations. Group-theoretical derivation of (5.2) and some consequences of the "accidental" degeneracy are given below.

** These states arise when the Sch. Eq. is solved for a Coulomb potential in parabolic coordinates. Note that the variables are separable in this case in the elliptic coordinates too. This possibility of the separation of variables in different coordinate systems is one of the consequences of accidental degeneracy; different coordinate systems correspond to different complete sets of commuting operators (commuting with the Hamiltonian and between themselves).

In a non-Coulombic potential, we may take a superposition of two solutions with different l, but these solutions will also have different energies. The time-dependent wave function therefore has the form (the subscript corresponds to l)

$$\psi(r, t) = \psi_0(r)\, e^{-\frac{iE_0 t}{\hbar}} + \psi_1(r)\, e^{-\frac{iE_1 t}{\hbar}}. \tag{5.5}$$

For $E_1 \neq E_0$ the dipole moment calculated using this wave function oscillates with a period of $\frac{2\pi\hbar}{E_1 - E_0}$, and the time-average dipole moment is identically zero.

Classical-mechanical arguments readily show why the Coulomb potential gives rise to a dipole moment.

Classical orbits in a Coulomb potential are Keplerian ellipses, with the source charge in one of the foci of the ellipse (Figure 3). At the "aphelion" (the farthest point) the electron moves more slowly than at the "perihelion" (the point closest to the proton). In case of Keplerian motion of the electron, the hydrogen atom on the average has a dipole moment; the time-averaged position of the electron r corresponds to a point on the semimajor axis lying midway between the center and the second focus of the ellipse.

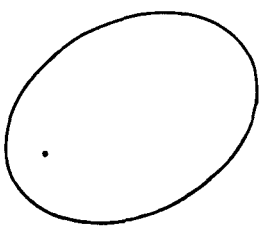

FIGURE 3.

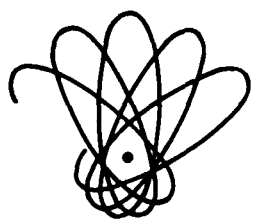

FIGURE 4.

Now consider the case of a non-Coulombic potential; for example, the potential set up by the sodium nucleus and the 10 inner electrons is not a Coulomb potential, so that the eleventh outermost valent electron in a sodium atom moves in a non-Coulombic potential. In a non-Coulombic field the classical orbit is not closed* (Figure 4), i.e., the major axis of the ellipse turns (precesses) around the focus. This classical picture is fully consistent with the quantum result: the dipole moment oscillates and averages out to zero in time.

The four wave functions with $n = 2$ can be chosen in a different way, so that each of the four orthogonal states has dipole moment of the same magnitude, the directions of the dipole moment vector corresponding to the four corners of a tetrahedron with the nucleus at its center.

* Note that according to Bertrand's theorem /31/, the Coulomb potential and the potential of a harmonic oscillator are the only spherical-symmetric potentials in the three-dimensional case which admit of closed orbits. (In this connection see the interesting remarks of Ehrenfest /32/ on the uniqueness of the three-dimensional case compared to other cases.)

Let l_i $(i = 1, 2, 3, 4)$ be the four three-dimensional unit vectors pointing from the center of the tetrahedron to its apexes: $l_i l_j = \frac{4}{3}\delta_{ij} - \frac{1}{3}$. We also introduce the following notation:

$$\psi_0 = \psi_{2,0,0},\ \boldsymbol{\psi} = (\psi_x,\ \psi_y,\ \psi_z),\ \psi_x = \frac{1}{\sqrt{2}}(\psi_{2,1,1} + \psi_{2,1,-1}),$$
$$\psi_y = \frac{1}{\sqrt{2}i}(\psi_{2,1,1} - \psi_{2,1,-1}),\ \psi_z = \psi_{2,1,0}.$$

It is now readily seen that the four functions

$$\psi_i = \frac{1}{2}(\psi_0 + \sqrt{3}\, l_i \boldsymbol{\psi}) \tag{5.6}$$

have the desired properties.

These wave functions (the so-called σ-electrons) are the zeroth approximation to the chemical bond of a carbon atom with other atoms. The carbon atom has precisely four electrons with $n = 2$. We know from organic chemistry that the covalent bonds of carbon are indeed directed to the four corners of a tetrahedron /33/.

We can now proceed with the derivation of (5.2). Our method will be somewhat unusual, as we will derive E_n by an entirely algebraic technique.* Note that Pauli /34/ derived this formula roughly in the same way long before the formulation of the Sch. Eq.

First note that (as we know from classical mechanics) the angular momentum vector is not the only conserved vector in a Coulomb field: the so-called Runge — Lenz vector /35, 36/, which is directed along the semimajor axis of the ellipse, is also conserved:**

$$\boldsymbol{A} = -\sqrt{m}\left(-\alpha\frac{\boldsymbol{r}}{r} + \frac{1}{m}[\boldsymbol{pL}]\right),\quad \alpha = \frac{Ze^2}{\hbar}. \tag{5.7}$$

It is readily seen that the operator

$$\hat{\boldsymbol{A}} = -\sqrt{m}\left(-\alpha\frac{\boldsymbol{r}}{r} + \frac{1}{2m}([\boldsymbol{pL}] - [\boldsymbol{Lp}])\right) \tag{5.8}$$

commutes with the Hamiltonian $[\hat{\boldsymbol{A}},\ H] = 0$, and therefore the operator $\hat{\boldsymbol{A}}$ is a quantum-mechanical generalization of the vector $\boldsymbol{A}$. The commutation relations for the operators L_i and A_j have the form

$$\left.\begin{aligned}&[L_i, L_j] = i\varepsilon_{ijk}L_k,\ [L_i, A_j] = i\varepsilon_{ijk}A_k,\\ &[A_i, A_j] = -2iH\varepsilon_{ijk}L_k.\end{aligned}\right\} \tag{5.9}$$

Let us now consider states with fixed negative energy. For these states we may treat $H = E$ as a constant negative number, replacing A_i by the operators $N_i = (-2H)^{-1/2}A_i$. Relations (5.9) take the form of commutation

* If the reader finds the following argument too abstruse, he can safely omit the remainder of this section.

** In a historical aside we should mention that this integral of motion was already known to Laplace /37/.

relations for the generators of the rotation group of the four-dimensional Euclidean space, $O(4)$ /38/:*

$$\left.\begin{aligned}&[L_i,\ L_j] = i\varepsilon_{ijk}L_k,\ [L_i,\ N_j] = i\varepsilon_{ijk}N_k,\\ &[N_i,\ N_j] = i\varepsilon_{ijk}L_k.\end{aligned}\right\} \tag{5.9'}$$

Note the following important identities satisfied by L_i and N_j:

$$\boldsymbol{LN} = \boldsymbol{NL} = 0,\ \boldsymbol{L}^2 + \boldsymbol{N}^2 + 1 = -\frac{E_0}{2H},\ E_0 = \frac{Z^2e^4m}{\hbar^2}. \tag{5.10}$$

At this stage we introduce two new vector operators

$$\boldsymbol{J}^{(1)} = \frac{1}{2}(\boldsymbol{L} + \boldsymbol{N}),\ \boldsymbol{J}^{(2)} = \frac{1}{2}(\boldsymbol{L} - \boldsymbol{N}), \tag{5.11}$$

commuting like the angular momentum operator for the three-dimensional rotation group $O(3)$; $\boldsymbol{J}^{(1)}$ and $\boldsymbol{J}^{(2)}$ also commute between themselves:

$$\left.\begin{aligned}&[J_i^{(1)},\ J_j^{(1)}] = i\varepsilon_{ijk}J_k^{(1)},\quad [J_i^{(2)},\ J_j^{(2)}] = i\varepsilon_{ijk}J_k^{(2)},\\ &[J_i^{(1)},\ J_j^{(2)}] = 0.\end{aligned}\right\} \tag{5.9''}$$

Hence it follows that the eigenvalues of $(\boldsymbol{J}^{(1,2)})^2$ are $j_{1,2}(j_{1,2}+1)$, and by (5.10)

$$(\boldsymbol{J}^{(1)})^2 = (\boldsymbol{J}^{(2)})^2 = \frac{\boldsymbol{L}^2 + \boldsymbol{N}^2}{4} = j(j+1),\ E = H = -\frac{E_0}{2(2j+1)^2}. \tag{5.12}$$

Comparison of (5.12) and (5.2) shows that

$$n = 2j + 1,\quad j = j_1 = j_2 = \frac{n-1}{2}. \tag{5.12'}$$

It also follows from the preceding that the degree of degeneracy is $(2j_1 + 1)(2j_2 + 1) = (2j + 1)^2 = n^2$.

We know that the transformation properties of functions under the group $O(4)$ — the four-dimensional rotation group — are completely determined by the numbers j_1 and j_2, i.e., the eigenvalues of the operators $(\boldsymbol{J}^{(1)})^2$ and $(\boldsymbol{J}^{(2)})^2$ (or the operators $\boldsymbol{L}^2 + \boldsymbol{N}^2$ and $\boldsymbol{LN}$). If j_1 and j_2 are known, we say that the functions are transformed according to the representation $D(j_1, j_2)$ of the group $O(4)$. In our case, the wave functions for a fixed $E = E_n$ transform according to the representation $D\left(\frac{n-1}{2}, \frac{n-1}{2}\right)$.

As we have noted before, in the degenerate case for a fixed energy $E < 0$ we may consider different systems of wave functions. For example, in the usual case of the separation of variables in spherical coordinates, the corresponding wave functions $\psi_{nlm}(\boldsymbol{r})$ are the eigenfunctions of the operators H, L^2 and L_z. We may consider, however, the eigenfunctions of the operators H, $J_z^{(1)}$, and $J_z^{(2)}$. These functions $\psi_{nk_1k_2}$ arise in the separation of variables in parabolic coordinates /40/; here k_1 and k_2 are related by the

* In the n-dimensional case, relations of the form (5.9) and (5.9') take the form of commutation relations for the generators of the group $O(n+1)$ /39/.

following equalities to the numbers n_1 and n_2, which are generally used with parabolic coordinates:

$$k_1 = \frac{1}{2}(m + n_1 - n_2),\ k_2 = \frac{1}{2}(m - n_1 + n_2),$$
$$-k \leqslant k_1,\ k_2 \leqslant k,\ k = \frac{n-1}{2};\ n_1 + n_2 + |m| + 1 = n.$$

Since $\boldsymbol{L} = \boldsymbol{J}^{(1)} + \boldsymbol{J}^{(2)}$ the transition from one method of description to another reduces to the famous problem of composition of two angular momenta $j_1 = j_2 = \frac{n-1}{2} = k$. Adding up these momenta we find that for a given n, l takes on values from 0 to $n-1$. It is also easily seen that ψ_{nlm} and $\psi_{nk_1k_2}$ are related by /41/

$$\left.\begin{aligned} \psi_{nlm} &= \sum_{k_1+k_2=m} (kk_1,\ kk_2|lm)\,\psi_{kk_1k_2}, \\ \psi_{kk_1k_2} &= \sum_{l=|m|}^{2k} (kk_1,\ kk_2|lm)\,\psi_{nlm}, \end{aligned}\right\} \tag{5.13}$$

where the numbers $(j_1m_1,\ j_2m_2|jm)$ are the Clebsch–Gordan coefficients.

We have thus established that the Sch. Eq. is invariant under the group of four-dimensional rotations, and that this invariance completely accounts for degeneracy of energy levels. Therefore, the term "accidental" degeneracy is not quite to the point.

We have so far concentrated on a somewhat formalistic treatment and made no attempt to determine the explicit form of the wave functions.

Let us now transform the Sch. Eq. following Fock /42, 43/ to a form invariant under $O(4)$. The Sch. Eq. in the momentum representation has the form

$$\left(\frac{p^2}{2m} - E\right)\psi(\boldsymbol{p}) - \frac{Ze^2}{2\pi^2\hbar}\int \frac{\psi(\boldsymbol{p}')\,d\boldsymbol{p}'}{|\boldsymbol{p}-\boldsymbol{p}'|^2} = 0. \tag{5.14}$$

We will consider the momentum space as a stereographic projection of a four-dimensional space, introducing new variables

$$\xi_0 = \frac{p_0^2 - p^2}{p_0^2 + p^2},\quad \boldsymbol{\xi} = \frac{2p_0\boldsymbol{p}}{p_0^2 + p^2};\quad \xi_0^2 + \boldsymbol{\xi}^2 = 1,\qquad p_0 = \sqrt{2m|E|},\quad E = -\frac{p_0^2}{2m}. \tag{5.15}$$

Changing over to a new wave function

$$\psi(\xi) = (p^2 + p_0^2)^2\psi(\boldsymbol{p}), \tag{5.16}$$

we obtain the equation

$$\psi(\xi) - \frac{\eta}{2\pi^2}\int \frac{d\xi'}{\xi_0'}\frac{\psi(\xi')}{(\xi-\xi')^2} = 0,\ \eta = \frac{\alpha m}{p_0}. \tag{5.17}$$

Fock has noted /42, 43/ that this is actually an equation for four-dimensional spherical functions $Y_{nlm}(\xi)$, and the corresponding values of the parameter η are thus equal to n. *

* It is clear that in case of attraction ($\eta > 0$), $E_n = -\frac{\alpha^2 m}{2n^2}$, and in case of repulsion ($\eta < 0$) no bound states are observed.

We have thus obtained the following result: the wave functions of the Coulomb problem have the form

$$\psi_{nlm}(p) = C_{nlm}(p^2 + p_0^2)^2 Y_{nlm}(\xi) \tag{5.18}$$

(here C_{nlm} is a normalization constant).

It is significant that the wave functions of the discrete spectrum turned to be proportional to four-dimensional spherical functions. The theory of these and general n-dimensional spherical functions is treated in considerable detail in /44, 45/, where the explicit form of these functions can be found.

Note that by using wave functions in the form (5.18) we can derive explicit expressions for certain sums encountered in the theory of the atom /42, 43/ and find an elegant representation of the Coulomb Green's function for $E < 0$ /46/.

The functions of the continuous spectrum have similar, though somewhat more complicated properties. The main distinction from the case of a discrete spectrum is that the four-dimensional sphere of our analysis is replaced by a four-dimensional two-sheet hyperboloid and the finite-dimensional representations of the $O(4)$ group are replaced by infinite-dimensional unitary representations of the Lorentz group. Detailed treatment of the continuous spectrum can be found in /47/. Note that similar symmetries are also observed for a Coulomb potential in n-dimensional space /47, 48/.

§ 6. THREE-DIMENSIONAL OSCILLATOR

Consider the potential

$$U = \frac{kr^2}{2}, \tag{6.1}$$

with $k > 0$. This potential does not satisfy the condition $U(\infty) = 0$. Therefore to real physical systems it is applicable only to some approximation, as long as r is not excessively large; at great distances, the real potential inevitably deviates from (6.1).

This potential is nevertheless used in nuclear physics, e.g., in the shell model of the nucleus /49/ and in the collective model /50, 51/.

An important property of this potential, which remains valid in the one-dimensional case too, is that its levels are equidistant. This leads to an immediate analogy between the excited state of a single oscillator with energy $(n + \frac{1}{2})\hbar\omega$ and the state of a system comprising n identical particles each of energy $\hbar\omega$. This analogy is the underlying basis of what is known as the "method of second quantization", which is concerned with processes involving a variable number of particles. In particular, various properties of electromagnetic radiation are found to coincide with the properties of an ensemble of quantum-mechanical oscillators.

Further, the radiation from a large system of two-level particles (this is the model generally used in the theory of lasers) can be reduced to the

radiation from one oscillator in many-dimensional space. The energy levels of this oscillator are degenerate, like the levels in a Coulomb potential. We will consider the case of "accidental" degeneracy for a three-dimensional oscillator.

The solution of the Sch. Eq. with potential (6.1) is sought in the form

$$\psi(r) = \psi_1(x_1)\,\psi_2(x_2)\,\psi_3(x_3). \tag{6.2}$$

Each of these functions satisfies the one-dimensional Sch. Eq. with a harmonic oscillator potential. The total energy is the sum of the energies corresponding to motion along the three coordinate axes,

$$\left.\begin{aligned} E = E_1 + E_2 + E_3, \quad E_l = \left(n_l + \tfrac{1}{2}\right)\hbar\omega, \\ E = (n_1 + n_2 + n_3 + \tfrac{3}{2})\hbar\omega, \quad \omega = \sqrt{\tfrac{k}{m}}. \end{aligned}\right\} \tag{6.3}$$

The energy levels of a three-dimensional spherically symmetric oscillator are thus degenerate. The general expression for the energy is

$$E_n = \left(n + \tfrac{3}{2}\right)\hbar\omega,$$

where n is an integer. The degree of degeneracy, i.e., the number of linearly independent solutions with the same energy, is equal to the number of ways in which n can be split into three non-negative integers. We construct an equilateral triangle with n units per side and draw a grid which divides the triangle into small triangles of unit side. The distance of each grid point from the sides of the large triangle is an integral number of heights of the unit triangles. The sum of these three integers is n. The degree of degeneracy N is thus equal to the total number of grid points, including those along the three sides of the large triangle (for these, one of the three quantum numbers is zero) and at its vertices (where two quantum numbers are zero and the third is n). The total number of grid points is readily seen to be equal to

$$N = \frac{(n+1)(n+2)}{2}. \tag{6.4}$$

According to a general theorem, the levels in a spherically symmetric potential $U = \frac{kr^2}{2}$ can be classified according to the orbital momentum l and its projection m.

A state defined in the form (6.2) by three quantum numbers n_1, n_2, n_3 in general does not have definite l and m. A useful exercise is therefore to observe how linear combinations of states of the form (6.2) give states with definite l and m.

For $n = 0$ there is but one state and it is readily seen to correspond to $l = 0$.

For $n = 1$ there are three states. It is readily verified that their linear combinations give precisely three states with $l = 1$. Here $\psi_0(x_1)\,\psi_0(x_2)\,\psi_1(x_3)$ is a state with $l = 1$, $m = 0$; $\frac{1}{\sqrt{2}}\,[\psi_1(x_1)\,\psi_0(x_2) \pm i\psi_0(x_1)\,\psi_1(x_2)]\,\psi_0(x_3)$ is a state with $l = 1$, $m = \pm 1$.

For $n = 2$ there are six states. They can be combined to form one state with $l = 0$ and five states with $l = 2$, m taking all values from 2 to -2.

In the general case, to each n corresponds a range of states with $l = n$, $l = n-2$, $l = n-4, \ldots$ up to $l = 1$ or $l = 0$, depending on the parity of n. Each l occurs once and only once.

In a three-dimensional oscillator, as in a Coulomb potential, levels with different l, say $l = 2$ and $l = 0$, are thus degenerate.

We will now show that in this case, as in the case of a Coulomb potential, the Sch. Eq. is invariant under a wider transformation group than the group of three-dimensional rotations /52 — 54/.

Consider the operators*

$$\left.\begin{aligned} a_l^+ = \frac{1}{\sqrt{2}}\left(\xi_l - \frac{d}{d\xi_l}\right), \quad a_l = \frac{1}{\sqrt{2}}\left(\xi_l + \frac{d}{d\xi_l}\right), \\ \xi_l = \frac{x_l}{x_0}, \quad x_0 = \sqrt{\frac{\hbar}{m\omega}}, \end{aligned}\right\} \tag{6.5}$$

which satisfy the commutation relations

$$[a_l, a_j^+] = \delta_{lj}, \quad [a_l, a_j] = [a_l^+, a_j^+] = 0. \tag{6.6}$$

The Hamiltonian now takes the form

$$H = \hbar\omega \sum_{l=1}^{3} \left(a_l^+ a_l + \frac{1}{2}\right) = \hbar\omega\left[\sum_{l=1}^{3} a_l^+ a_l + \frac{3}{2}\right]. \tag{6.7}$$

It is readily seen that the Hamiltonian (6.7) is invariant under the unitary transformation

$$a_l \to a_l' = \sum_{j=1}^{3} u_{lj} a_j, \quad a_l^+ \to a_l'^+ = \sum_{j=1}^{3} u_{lj}^* a_j^+, \tag{6.8}$$

or, in other words, the Hamiltonian of a three-dimensional oscillator is invariant under the group of third-order unitary matrices, the $U(3)$ group. The corresponding group for the n-dimensional oscillator is readily seen to be the group $U(n)$.

We now introduce the operators $A_l^j = a_j^+ a_l$. They commute with the Hamiltonian, $[A_l^j, H]$, and also satisfy the following commutation relations:

$$[A_l^j, A_k^i] = \delta_l^i A_k^j - \delta_k^j A_l^i. \tag{6.9}$$

These relations coincide with the known commutation relations for the generators of the $U(3)$ group /55, 56/, whence the conclusion that A_l^j is a generator of this group.

Consider the combination

$$A = \sum_{l=1}^{3} A_l^l = \frac{1}{\hbar\omega} H - \frac{3}{2}.$$

* If you are familiar with quantum field theory, you will readily recognize in these operators the creation and destruction operators of oscillation quanta.

Since A for obvious reasons commutes with H and with all A_i^j, it is worthwhile to separate it from the other six operators A_i^j.

We thus introduce new operators

$$B_i^j = A_i^j - \frac{1}{3}\delta_i^j A, \quad \sum_i B_i^i = 0. \tag{6.10}$$

These nine new operators, eight of which are independent, commute as before, but on account of the identity $\Sigma B_i^i = 0$ they are generators of $SU(3)$, the group of third-order unitary matrices with unit determinant.* Note that the usual rotation group, $O(3)$, is contained as a subgroup in $SU(3)$. The representations of $SU(3)$ are well known: they are fully characterized by two numbers p and q. However, not all the representations of this group are realized by oscillator wave functions. Indeed, as our problem is concerned only with one species of operators a_i, we can form only functions of the symmetric tensor type. These functions are transformed according to the representation $D(p, q)$ with $p = n$, $q = 0$. The degeneracy and the range of the orbital momenta l in a state with given energy can therefore be derived from the general relations of group theory. The treatment on p. 23, however, is quite sufficient for our purposes.

Note that accidental degenracy is directly responsible for the fact that the classical path of an oscillator is a closed curve — an ellipse centered at the origin.

What is the reason for the relation between the closed classical paths and degenerate levels with various l? A classical particle occupying a definite point with definite values of the angular variables θ and φ is described in quantum mechanics by a wave packet, i.e., a superposition of states with various l. In the nondegenerate case, the phase relations between the states with various l change in time and the wave packet gradually spreads in space in accordance with the classical conception of motion in a trajectory of the form shown in Figure 4.

Note that the degeneracy of levels with various m for a given l, which is observed in any spherical-symmetric potential, corresponds to the classical theory of the exact conservation of the orbital plane.

A characteristic distinction between the degeneracy in an oscillator and the Coulomb degeneracy is that the degenerate levels in an oscillator have the same parity, equal to the parity of n.

To establish this point, note that the solutions of the one-dimensional problem have a definite parity, equal to $(-1)^n$ ($n = 1, 2, 3, \ldots$).

It follows from the preceding that a superposition of oscillator states with different l but equal energy also has a definite parity, so its dipole moment is zero. It is thus impossible to form a stationary state with $d \neq 0$. This conclusion is also quite understandable from the classical standpoint, as the oscillator trajectory is symmetric about the origin.

Finally let us consider the case of a one-dimensional oscillator in application to the so-called problem of "coherent states" (we follow the treatment of /60/). Various important properties of these states were studied in Glauber's classical paper /61/, to which the reader is referred for further details.

* This group is being currently used as the symmetry group of strongly interacting particles /57, 58/; numerous theoretical problems associated with this group were therefore resolved by physicists. Analogy between the symmetry of strongly interacting particles and the symmetry of the oscillator is discussed in Dyson's remarkable paper /59/.

What makes the coherent states particularly important? The main feature, as we shall see in the following, is that their properties are very close to the classical properties. Introduction of these states apparently provides the most natural description of the coherent properties of a light beam (e.g., a laser beam) in quantum mechanics. These states are also useful for treatment of soft quanta.

Let the oscillator be in some state n, where it is described by wave function ψ_n. Following Dirac /62/, we designate this state by $|n\rangle$. States of this kind, i.e., the conventional stationary states, are not suitable for passing from quantum mechanics to classical mechanics, as the mean coordinates and the mean momentum in these states vanish, *

$$x_n(t) = \langle n|\hat{x}|n\rangle = 0,\ p_n(t) = \langle n|\hat{p}|n\rangle = 0, \tag{6.11}$$

whereas in classical mechanics

$$x(t) = A\cos(\omega t - \varphi). \tag{6.12}$$

Let us try to find a state $|\psi_{cl}\rangle$ such that

$$x(t) = \langle \psi_{cl}(t)|\hat{x}|\psi_{cl}(t)\rangle. \tag{6.13}$$

A suitable state is found to have the form**

$$|\alpha\rangle = e^{-\frac{\rho^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle,\ \rho = |\alpha|. \tag{6.14}$$

The average number of oscillation quanta in this state is

$$\bar{n} = \frac{\langle \alpha|a^+a|\alpha\rangle}{\langle \alpha|\alpha\rangle} = \rho^2, \tag{6.15}$$

and the probability P_n of finding an oscillator in the state $|n\rangle$ is given by the usual Poisson distribution

$$P_n(\alpha) = e^{-\rho^2}\frac{\rho^{2n}}{n!} = e^{-\bar{n}}\frac{\bar{n}^n}{n!}. \tag{6.16}$$

It is further readily seen that in this case

$$(\Delta x)^2 = \overline{x^2} - \bar{x}^2 = \frac{\hbar}{2m\omega},\ (\Delta p)^2 = \overline{p^2} - \bar{p}^2 = \frac{m\hbar\omega}{2},$$

whence

$$\Delta x \cdot \Delta p = \frac{\hbar}{2}, \tag{6.17}$$

i.e., the uncertainty relation for the coordinate and the momentum has its minimum value in this case.

* This is the general property of stationary states of the discrete spectrum.

** These states were first considered by Schroedinger /63/.

We will now prove our propositions. Expression (6.13) can be rewritten in the form

$$x(t) = \langle \psi_{cl}(0) | \hat{x}(t) | \psi_{cl}(0) \rangle = \\ = x_0 \langle \psi_{cl}(0) | ae^{-i\omega t} + a^+ e^{i\omega t} | \psi_{cl}(0) \rangle; \qquad (6.13')$$

here

$$\hat{x}(t) = e^{i\hat{H}t} \hat{x} e^{-i\hat{H}t} = \frac{x_0}{\sqrt{2}} (ae^{-i\omega t} + a^+ e^{i\omega t}), \quad x_0 = \sqrt{\frac{\hbar}{m\omega}}.$$

It is readily seen that condition (6.13) is satisfied for states $|\alpha\rangle$ such that

$$a|\alpha\rangle = \alpha|\alpha\rangle, \qquad (6.18)$$

where $\alpha = \rho e^{i\varphi}$ is a complex number.

Indeed, for such a state we have

$$\langle \alpha | \hat{x}(t) | \alpha \rangle = \frac{x_0}{\sqrt{2}} (\alpha e^{-i\omega t} + \alpha^* e^{i\omega t}) \langle \alpha | \alpha \rangle = \sqrt{2} x_0 \rho \langle \alpha | \alpha \rangle \cos(\omega t - \varphi). \qquad (6.19)$$

We now expand the state $|\alpha\rangle$ in states $|n\rangle$:

$$|\alpha\rangle = \sum_{n=0}^{\infty} \langle n | \alpha \rangle |n\rangle. \qquad (6.20)$$

Left-multiplying (6.18) by $\langle n|$ and using the identity $\langle n|a = \sqrt{n+1}\,\langle n+1|$, we find

$$\langle n+1 | \alpha \rangle = \frac{\alpha}{\sqrt{n+1}} \langle n | \alpha \rangle,^*$$

so that

$$\langle n | \alpha \rangle = \frac{\alpha^n}{\sqrt{n!}} \langle 0 | \alpha \rangle, \quad |\alpha\rangle = \langle 0|\alpha\rangle \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle. \qquad (6.21)$$

$\langle 0|\alpha\rangle$ is found from the normalization condition for the state $|\alpha\rangle$:

$$\langle \alpha | \alpha \rangle = 1, \quad |\langle 0|\alpha\rangle|^2 \sum_{n=0}^{\infty} \frac{\rho^{2n}}{n!} = |\langle 0|\alpha\rangle|^2 e^{\rho^2} = 1,$$

whence follows (6.14).

It is now clear that the eigenvalue α has the form $\alpha = (\bar{n})^{1/2} e^{i\varphi}$. It would therefore seem that there exists a representation $\hat{a} = (\hat{n})^{1/2} e^{i\hat{\varphi}}$, where $\hat{\varphi}$ is a Hermitian operator; it was shown in /64/, however, that no such operator exists.

We now substitute in (6.14) $|n\rangle = \frac{(a^+)^n}{\sqrt{n!}}|0\rangle$; then

$$|\alpha\rangle = e^{-\frac{\rho^2}{2}} \sum_{n=0}^{\infty} \frac{(\alpha a^+)^n}{n!} |0\rangle = e^{-\frac{\rho^2}{2} + \alpha a^+} |0\rangle. \qquad (6.22)$$

* This identity is readily obtained from the fundamental equality $|n\rangle = \frac{1}{\sqrt{n!}} (a^+)^n |0.\rangle$.

We have obtained a simple expression for the operator which transforms $|0\rangle$ into $|\alpha\rangle$. This operator, however, is not unitary. Consider the unitary operator

$$A(\alpha) = e^{\alpha a^+ - \alpha^* a}. \tag{6.23}$$

Using Baker and Hausdorf's famous identity /65, 66/

$$e^A \cdot e^B = e^{\left\{A+B+\frac{1}{2}[A,B]\right\}}, \tag{6.24}$$

which is valid when $[A[A, B]] = [B[A, B]] \simeq 0$, and putting $A = \alpha a^+, B = -\alpha^* a$, $[A, B] = |\alpha|^2 = \rho^2$, we obtain

$$A(\alpha) = e^{\alpha a^+ - \alpha^* a} = e^{-\frac{\rho^2}{2}} e^{\alpha a^+} \cdot e^{-\alpha^* a}, \tag{6.25}$$

whence it follows directly that $|\alpha\rangle = A(\alpha)|0\rangle$.

Note that the operators $A(\alpha)$ have the following properties:

$$\left.\begin{aligned} &A(\alpha) = A^+(-\alpha),\ A^+(\alpha)A(\alpha) = A(\alpha)A^+(\alpha) = 1, \\ &A(-\alpha)A(\alpha) = A(\alpha)A(-\alpha) = 1, \quad A(-\alpha)|\alpha\rangle = |0\rangle. \end{aligned}\right\} \tag{6.26}$$

It is also readily seen that

$$\left.\begin{aligned} &[a,\ A(\alpha)] = \alpha A(\alpha), \\ &A^+(\alpha) a A(\alpha) = a + \alpha,\ A^+(\alpha) a^+ A(\alpha) = a^+ + \alpha^*. \end{aligned}\right\} \tag{6.27}$$

Finally, let us consider the orthogonality and the completeness of the coherent states. We have

$$\left.\begin{aligned} &\langle\alpha|\beta\rangle = e^{-\frac{1}{2}(|\alpha|^2+|\beta|^2)} \sum_{n=0}^{\infty} \frac{(\alpha^*\beta)^n}{n!} = e^{-\frac{1}{2}(|\alpha|^2+|\beta|^2-2\alpha^*\beta)}, \\ &|\langle\alpha|\beta\rangle|^2 = e^{-|\alpha-\beta|^2}. \end{aligned}\right\} \tag{6.28}$$

These states are thus not orthogonal to one another. They nevertheless constitute a complete system of states. This can be verified by taking the integral

$$\int d^2\alpha\, |\alpha\rangle\langle\alpha|, \text{ where } \alpha = \alpha_1 + i\alpha_2 = \rho e^{i\varphi},\ d^2\alpha = d\alpha_1\, d\alpha_2.$$

Inserting for $|\alpha\rangle$ its expression from (6.14), we find

$$\int d^2\alpha\, |\alpha\rangle\langle\alpha| = \int \rho\, d\rho \int d\varphi\, \frac{|m\rangle\langle n|}{\sqrt{m!n!}} e^{-\rho^2} \rho^{m+n} e^{i(m-n)\varphi} =$$
$$= \pi \sum_{m=0}^{\infty} |m\rangle\langle m| \frac{1}{m!} \int d\rho^2 \rho^{2m} e^{-\rho^2} = \pi \sum_{m=0}^{\infty} |m\rangle\langle m|.$$

We thus have the equality

$$\frac{1}{\pi} \int d^2\alpha\, |\alpha\rangle\langle\alpha| = \sum_{n=0}^{\infty} |n\rangle\langle n|, \tag{6.29}$$

which is in fact the completeness condition for a system of states. Using this equality, we can expand any state in terms of the coherent states $|\alpha\rangle$.

In conclusion note that coherent states can be applied to derive without difficulty a closed expression for the transition probability of an oscillator between two states in an arbitrary external field /60/.

§ 7. THE VIRIAL THEOREM AND ITS GENERALIZATIONS

Coulomb and oscillator potentials are particular cases of the general power potential $U = kr^n$. For these potentials we have the virial theorem* which establishes a relation between the average kinetic and potential energy.

Following Fock /69/, we will first derive this theorem from the variational principle.

According to the variational principle, the expectation value of the operator H for the eigenstate ψ_n of H with the eigenvalue E_n is stationary. In other words, if

$$H\psi_n = E_n \psi_n,$$

then $\overline{H} = \int \psi^* H \psi \, d\boldsymbol{r}$ or, better still,**

$$\overline{H} = \frac{\int \psi^* H \psi d\boldsymbol{r}}{\int \psi^* \psi d\boldsymbol{r}} \tag{7.1}$$

for $\psi = \psi_n + \delta\psi$ differs from E_n by terms of the order $(\delta\psi)^2$; terms of the order $\delta\psi$ vanish. In particular, for ψ_0 corresponding to the lowermost (ground) state the assertion is that the substitution $\psi = \psi_0$ gives an absolute minimum $\overline{H} = E_0$.

The variational principle is best verified by expanding the variation in eigenfunctions of the operator H:

$$\delta\psi = \sum_m \delta C_m \psi_m;$$

using the orthogonality of the eigenfunctions, we find that the variation of $\overline{H}$ is proportional to $(\delta C_m)^2$.

We now write $\overline{H} = \overline{U} + \overline{T}$, where $\overline{U}$ is the expectation value of the potential energy, $\overline{T}$ the kinetic energy expectation value.

Consider a special kind of variation of ψ, namely an infinitesimal similarity transformation

$$\psi' = \psi + \delta\psi = \left(1 + \frac{3}{2}\varepsilon\right)\psi[(1+\varepsilon)\boldsymbol{r}], \tag{7.2}$$

where ε is a small quantity. The factor before ψ ensures that the normalization is conserved, $\int |\psi'|^2 d\boldsymbol{r}' = \int |\psi|^2 d\boldsymbol{r}$.

Since $\overline{U} = k\overline{r^n}$, we clearly have $\frac{\delta\overline{U}}{\overline{U}} = -n\varepsilon$.

* In classical mechanics, this theorem was already known to Clausius. In quantum mechanics it was first established by Born, Heisenberg, and Jordan /67/. Various formulations of the virial theorem and its generalization to the case of a continuous spectrum can be found in /68/.

** In (7.1) there is no need to be concerned about the normalization of the wave function being varied.

The kinetic energy is proportional to $\int|\nabla\psi|^2 dr$ so that contraction of all distances increases the kinetic energy in inverse proportion to the square of the contraction factor $\frac{\delta\overline{T}}{\overline{T}} = 2\varepsilon$.

We now demand that $\delta\overline{H} = \delta\overline{U} + \delta\overline{T} = (-n\overline{U} + 2\overline{T})\varepsilon$ be extremum. Hence

$$\overline{T} = \frac{n}{2}\overline{U},\ \overline{H} = \frac{n+2}{2}\overline{U} = \frac{n+2}{n}\overline{T}, \tag{7.3}$$

which is the virial theorem. For a harmonic oscillator $\overline{T} = \overline{U}$, and for a Coulomb interaction the total energy H in a stationary state is equal to the mean kinetic energy with minus sign.

The variational principle provides a vivid answer to the question, "why the electron does not fall to the nucleus?" As the electron approaches the nucleus, its potential energy being proportional to $1/r$ decreases (the absolute value of the negative potential energy increases), but in virtue of the uncertainty principle the electron momentum grows as $1/r$, so that the kinetic energy increases as $1/r^2$. The total energy therefore has a minimum at a well defined average distance of the electron from the nucleus: further approach ("fall") of the nucleus is precluded by excessive growth of kinetic energy.

We see from the preceding that for potentials which increase faster than $1/r^2$ for $r \to 0$, the Sch. Eq. cannot have a definite ground level, and in this potential the particle will fall to the attracting center.

Another method for the derivation of the virial theorem is based on calculation of the mean value of $\frac{d}{dt}(\boldsymbol{rp}) = \frac{i}{\hbar}[H, \boldsymbol{rp}]$. It is readily seen that in a stationary state $\frac{d}{dt}\langle\boldsymbol{rp}\rangle = \frac{i}{\hbar}\langle[H, \boldsymbol{rp}]\rangle = 0$; moreover, an analogous expression obtains for any operator A:

$$\langle\dot{A}\rangle = \frac{i}{\hbar}\langle[H, A]\rangle = 0. \tag{7.4}$$

This is a generalization of the virial theorem /70/. A nontrivial aspect of the whole procedure is the choice of an appropriate operator A. A clever choice may lead to some remarkable relations for mean values.

We will apply the generalized virial theorem to Coulomb and harmonic potentials /71/. The Coulomb Hamiltonian can be written in the form

$$H = \frac{p_r^2}{2m} + \frac{\hbar^2\hat{L}^2}{2mr^2} - \frac{\alpha}{r}, \tag{7.5}$$

where

$$p_r = -i\frac{\hbar}{r}\frac{\partial}{\partial r}r = -i\hbar\left(\frac{\partial}{\partial r} + \frac{1}{r}\right),\ [p_r, r] = -i\hbar,$$

$$\dot{r} = \frac{p_r}{m},\ \dot{p}_r = \frac{\hbar^2\hat{L}^2}{mr^3} - \frac{\alpha}{r^2}.$$

For the operator A we choose $p_r r^{s+1}$. Equality (7.4) now takes the form

$$\frac{d}{dt}\overline{\langle p_r r^{s+1}\rangle} = \langle\dot{p}_r r^{s+1}\rangle + \langle p_r\dot{r}r^s\rangle + \ldots + \langle p_r r^s\dot{r}\rangle. \tag{7.6}$$

In (7.6) the operator $r = \frac{p_r}{m}$ can be moved to the left using the identity

$$r^k p_r = p_r r^k + i\hbar k r^{k-1}, \tag{7.7}$$

and this gives

$$\langle \dot{p}_r r^{s+1} \rangle + \frac{s+1}{m} \langle p_r^2 r^s \rangle + \frac{is(s+1)}{2} \frac{\hbar}{m} \langle p_r r^{s-1} \rangle = 0. \tag{7.6'}$$

To simplify the last term in this expression, consider the equality $\langle \dot{r}^s \rangle = 0$ or

$$\begin{gathered} \frac{s}{m} \langle p_r r^{s-1} \rangle + i \frac{s(s-1)}{2} \frac{\hbar}{m} \langle r^{s-2} \rangle = 0, \\ \langle p_r r^{s-1} \rangle = -i(s-1) \frac{\hbar}{2} \langle r^{s-2} \rangle. \end{gathered} \tag{7.8}$$

Expressing $\dot{p}_r$ and p_r^2 in terms of r by (7.5) and making use of (7.8), we find

$$2E(s+1)\langle r^s \rangle + \alpha(2s+1)\langle r^{s-1} \rangle + \frac{s\hbar^2}{m} \left(\frac{s^2-1}{4} - l(l+1) \right) \langle r^{s-2} \rangle = 0. \tag{7.9}$$

We have thus obtained a recursion formula for the mean values of the powers of r. This relation was originally derived by Kramers /72/ using a different method. Note that for $s = 0$, (7.9) yields the ordinary virial theorem and the term $\frac{\hbar^2 s(s^2-1)}{4m} \langle r^{s-2} \rangle$ allows for the fact that the operators r and p_r do not commute. Therefore its omission gives recursion expressions for the classical case.

Let us now consider the case of a three-dimensional harmonic oscillator. Here

$$H = \frac{1}{2m} p_r^2 + \frac{\hbar^2}{2m} \frac{\hat{L}^2}{r^2} + \frac{m}{2} \omega^2 r^2. \tag{7.10}$$

It is easily seen that relations (7.6)—(7.8) are valid as before. Expressing $\dot{p}_r$ and p_r^2 in terms of r from (7.10) and substituting in (7.6'), we obtain

$$2E(s+1)\langle r^s \rangle - m\omega^2 (s+2)\langle r^{s+2} \rangle + \frac{\hbar^2}{m} s \left[\frac{s^2-1}{4} - l(l+1) \right] \langle r^{s-2} \rangle = 0. \tag{7.11}$$

As in the previous case, $s = 0$ yields the virial theorem. Note that unlike (7.9), relations (7.11) include only odd or only even powers of r. This is not surprising, since the Hamiltonian (7.10) is even with respect to r, i.e., it does not change on substitution $r \to -r$.

§ 8. IDENTICAL PARTICLES AND STATISTICAL PHYSICS

The problem of motion of two interacting particles is reduced to a one-particle problem in quantum, as well as classical mechanics.

Therefore the Sch. Eq. with ψ dependent on the three coordinates is applicable not only to the motion of electron in the field of a heavy fixed nucleus, but also to the motion of a diatomic molecule. In this case we

use Born's and Oppenheimer's approximation: for given position of the nuclei, the electrons are assumed to occupy the lowermost energy state. The energy of the entire system, including the energy of the electrons, which depends on the distance between the nuclei, is regarded as an effective potential in which the nuclei move.

The solution of the Sch. Eq. for a diatomic molecule has the form $R(r)\,Y_{lm}(\theta, \varphi)$, where r, θ, φ characterize the vector r_{12} from nucleus 1 to nucleus 2.

A novel situation arises if the two nuclei are identical, as in the molecules H_2, C_2, N_2, O_2.

If the nuclei comprise an even number of nucleons, the wave function should be symmetric: these nuclei are called bosons, as they follow Bose statistics.

The situation is particularly simple if the nuclear spin is 0. As the wave function is symmetric under interchange of 1st and 2nd nuclei, i.e., under sign inversion $r_{12} \to -r_{12}$ (in this transformation $r \to r, \theta \to \pi - \theta, \varphi \to \varphi + \pi$), the odd values of l are excluded.

Experiments show that a C_2 molecule comprising two C^{12} nuclei may occupy only states with $l = 0$, $l = 1$, $l = 2$, $l = 4$, etc. A carbon molecule comprising two different nuclei C^{12}, C^{13} or C^{12}, C^{14} may occupy all the odd and even states $l = 0$, $l = 1$, $l = 2$, $l = 3$, etc.

Sometimes the difference between the classical (Boltzmann) statistics and the quantum statistics of Bose and Einstein is formulated as a difference in the method of counting of states.

Consider two particles A, B and two states 1, 2. In classical statistics we distinguish between two states: A_1B_2 and B_1A_2; in quantum statistics, if A and B are identical, the system has only one state, with one of the particles in state 1 and the other in state 2.

The carbon molecule $C^{12}C^{12}$ provides an excellent example: here clearly the quantum-statistical properties have nothing to do with the method of counting. In this Bose system, certain states (those with even l) are forbidden and do not occur in nature, although they do exist in systems comprising different particles. For identical particles we have an entirely different mechanics, which forbids certain states; the different statistics is simply a consequence of the different mechanics.

For fermions the situation is simpler, and even a novice is in no danger of committing an error: that no two particles may occupy the same state is an obvious restriction.

The situation which is fairly clear for a diatomic molecule is not so transparent for independent particles in a general field and especially not for a continuous spectrum. In the above example, for different A and B we are dealing with two different states A_1B_2 and B_1A_2. If A and B have close properties, the energy of these two states is nearly equal. Moreover, if A and B interact, the solutions of the Sch. Eq. are the combination states

$$A_1B_2 + B_1A_2 \quad \text{and} \quad A_1B_2 - B_1A_2.$$

Interaction mixes the original states, but according to general theorems it does not affect the overall number of states ($2 = 2$), just as rotation of the coordinate axes does not affect the dimension of space.

If the two particles A and B are two identical bosons $B = A$, only the symmetric state $A_1B_2 + B_1A_2$ exists; the second, antisymmetric state is forbidden in the same sense as $C^{12}C^{12}$ with $l = 1$ cannot exist. For fermions the symmetric (even) state $A_1B_2 + B_1A_2$ is forbidden and $A_1B_2 - B_1A_2$ exists.

In classical statistics the states are counted as if all the particles were different.

Let the number of particles be much less than the number of levels which are occupied on the average by these particles. The probability of finding two particles on one level (which is strictly forbidden for fermions) is therefore small. In this case, the total number of states for different particles differs from the number of states for bosons (or the equal number of states for fermions) by a constant factor $N!$, where N is the number of particles. The constant factor in the number of states introduces a constant term to the entropy and the free energy; classical statistics therefore leads to correct thermodynamic results in this case. The observable quantities, which are independent of the additive constant in Bose and Fermi statistics, will coincide with the results of classical statistics in the limit of low occupancy.

How are we to reconciliate the classical statistics with the fact that half the levels in a diatomic molecule are missing? To this end a molecular symmetry number 2 is introduced (for a diatomic molecule) and the phase volume is divided by 2 (or alternatively $k\ln 2$ is subtracted from the entropy).

It is interesting to trace the origin of the same number 2 in a diatomic molecule with nuclei of spin 1/2, e.g., H_2. The wave function in this case is representable as a product of orbit and spin functions.

The antisymmetric spin function $\alpha_1\beta_2 - \alpha_2\beta_1$ of two spin 1/2 particles corresponds to zero total spin. The symmetric function corresponds to $s = 1$: there are three such functions: $s_z = 1$, $\alpha_1\alpha_2$; $s_z = 0$, $\alpha_1\beta_2 + \alpha_2\beta_1$; $s_z = -1$, $\beta_1\beta_2$. For $s = 0$ the orbit function is even, $l = 0$, $l = 2, \ldots$ (para-hydrogen). For $s = 1$ the orbit function is odd, $l = 1$, $l = 3, \ldots$ (ortho-hydrogen). Thus, some rotational states have one spin state, $g = 1$, while others have three spin states, $g = 3$, the average being $\bar{g} = 2$.

A molecule comprising two different atoms, e.g., HT (a hydrogen—tritium molecule), has four spin states* for each l; for any l there is both $s = 0$, $g = 1$ and $s = 1$, $g = 3$.

The drop from $g = 4$ for a molecule comprising different atoms to $\bar{g} = 2$ for a molecule made up of identical atoms actually corresponds to the symmetry number 2.

The introduction of the symmetry number enables the classical statistics to cope successfully and correctly with various problems in the theory of molecular dissociation and in general with problems involving low occupancy numbers; in such systems the results are independent of spins and nuclear statistics; the results are further independent, as can be shown, of the fact whether we are dealing with a single species of nuclei or with an isotopic mixture.

One cannot expect correct results without clearly understanding the very foundations of classical, Bose and Fermi statistics, as elucidated (we hope) by the examples of this section.

* Note that these four states can be counted simply as a product of the two states of H ($s_z = +1/2$, $s_z = -1/2$) with the same two states of T. The total-spin classification does not alter the position.

Chapter 2

THE CONTINUUM

§ 9. INTRODUCTION. CONTINUUM WAVE FUNCTIONS WITH $l = 0$

In this chapter we consider states which form a continuum. These states, as we know, describe particle scattering in a potential field. The theory of scattering is an important subject in quantum mechanics which has been developed in considerable detail. The most comprehensive treatment of this theory can be found in Landau and Lifshitz's book /8/ and in the recently published monograph by Goldberger and Watson /73/, which is devoted in its entirety to collision theory. The latter book also gives a detailed bibliography on the subject. Here we will discuss only some of the properties of wave functions forming a continuous spectrum.

First consider continuum functions with given E and l. These functions, as it follows from (1.8), are essentially different from zero in the entire space. The condition of vanishing at infinity therefore does not apply and we are left only with condition (1.7) imposed on the two linearly independent functions $\chi^{(\pm)}$. Hence, for a fixed energy E and any l, we may form a solution which satisfies condition (1.7); furthermore, a r e a l solution may be chosen. Some properties of this solution for $l = 0$ are considered in the present section, and the case $l \neq 0$ is treated in § 10.

In the case of a continuum, as opposed to the case of a discrete spectrum, the Sch. Eq. has solutions for all l for a given $E > 0$. Therefore any superposition of these solutions is again a solution of the Sch. Eq., and vice versa: any solution of the Sch. Eq. with a definite positive energy can be represented as a superposition of solutions with different l and fixed E. It is because of this property that we can choose different complete systems of wave functions.

An important state frequently encountered in the theory of scattering is a superposition of a plane transmitted wave plus a scattered wave, i.e., a state whose asymptotic behavior for $r \to \infty$ is described by $e^{ikz} + f(\theta, \varphi)e^{+ikr}/r$. We can also form states with the asymptotics $e^{ikz} + f_1(\theta, \varphi)\, e^{-ikr}/r$; here the function $f_1 e^{-ikr}/r$ describes an incoming wave and e^{ikz} describes a particle emerging in the direction of the z axis. These functions, however, are encountered relatively seldom. The topics relating to this problem are treated in § 11.

Finally the last section (§ 12) of this chapter gives a derivation of the so-called optical theorem and its generalization is considered.

Let us now proceed with a more detailed discussion of states with fixed E and l. We will want to identify the states $\chi^{(\pm)}$. In a state described

by a function $\psi(r)$, the current of particles at a point r is given by

$$j(r) = -\frac{i\hbar}{2m}(\psi^*\nabla\psi - \psi\nabla\psi^*). \tag{9.1}$$

Inserting the functions $\frac{1}{\sqrt{4\pi}}\frac{\chi^{(\pm)}}{r}$, we find

$$j^{(\pm)}(r) = \pm\frac{v}{4\pi}\frac{r}{r^3}, \tag{9.2}$$

where $v = \frac{\hbar k}{m}$ is the velocity corresponding to the wave vector k. Thus, the function $\chi_k^{(+)}$ describes particles which move with velocity v in all directions from the origin (a divergent outgoing wave) and the function $\chi_k^{(-)}$ describes particles which move with velocity v toward the origin (a convergent incoming wave). The total incoming ($\chi^{(-)}$) or outgoing ($\chi^{(+)}$) flux of particles crossing a sphere of radius R every second is clearly given by

$$4\pi R^2 j^{(\pm)}(R) = \pm v. \tag{9.3}$$

The normalization of the functions $\chi_k^{(\pm)}$ used in (1.8) thus corresponds to the fact that v particles pass every second through a large sphere, the particle density ρ being $1/4\pi R^3$ particles/cm^3. Hence it follows that the functions $\chi^{(\pm)}$ are not solutions of the Sch. Eq. for $r = 0$, as this point is a source or sink of particles. The two functions $\chi_k^{(\pm)}$, however, can be formed into a linear combination $\chi_k(r)$ which shows proper behavior at $r = 0$. According to (1.9), χ_k includes both $\chi_k^{(-)}$ and $\chi_k^{(+)}$. The former corresponds to an incoming flux of particles falling on the force center from infinity, and the latter represents the outgoing flux. In other words, $\chi_k(r)$ describes the scattering of particles in a potential field $V(r)$.

Let us consider in more detail the case $l = 0$. The potential is assumed to be identically zero. The solutions

$$\chi_k^{(\pm)}(r) = e^{\pm ikr} \tag{9.4}$$

are then exact solutions of equation (1.6') in the entire space, except the point $r = 0$. The boundary conditions at $r = 0$ are satisfied by the unique solution

$$\varkappa_k(r) = \chi_k^{(-)} - \chi_k^{(+)} = -2i\sin kr \underset{r\to 0}{\longrightarrow} -2ikr. \tag{9.5}$$

Zero potential clearly leads to zero scattering. Therefore χ_k describes free, unperturbed motion of particles in space (with zero orbital momentum relative to $r = 0$). The coefficient $A(k)$ in

$$\chi_k = A(k)(\chi_k^{(+)} - S(k)\varkappa_k^{(+)})$$

(this is the amplitude of the incoming wave) is clearly an arbitrary parameter independent of the potential $U(r)$; $A(k)$ depends only on the number of particles "aimed" at $r = 0$ from infinity. $S(k)$, on the other hand, is determined entirely by the form of the potential, and it is this function that specifies the scattering power of the potential.

To isolate the part of the wave function which describes actual scattering in a potential field, we write $\chi_k(r)$ in the form

$$\chi_k(r) = A(k)\,[\chi_k^{(-)} - \chi_k^{(+)} - (S(k) - 1)\chi_k^{(+)}]. \tag{9.6}$$

The first two terms in brackets coincide for $r > R$ with the wave function of free motion (see (9.5)). The last term is therefore the one describing the scattered wave.

Scattering by a potential cannot involve absorption or creation of particles. Therefore the number of incident particles hitting the force center should be equal to the number of outgoing particles. In other words $|S(k)| = 1$ and we can always write $S(k)$ in the form

$$S(k) = e^{2i\delta(k)}, \tag{9.7}$$

where δ is a real function, called the scattering phase. In free motion we clearly have $\delta(k) = 0$ (see (9.6)). In general $\delta \neq 0$, and the wave function for $r \geqslant R$ can always be written in one of the following forms:

$$\begin{aligned}\chi_k(r) &= Ae^{i\delta}(\chi_k^{(-)}e^{-i\delta} - \chi_k^{(+)}e^{i\delta}) = \\ &= -2iAe^{i\delta}\sin(kr + \delta) = -2iA\,[\sin kr + e^{i\delta}\sin\delta e^{ikr}].\end{aligned} \tag{9.8}$$

What was our justification for splitting up the wave function into two parts and assigning them the meaning of wave functions for the incoming and the outgoing flux of particles? The question can be phrased differently. For a continuum of states a real wave function can always be chosen. We know, however, that in states described by a real wave function, the particle current is zero. Were we right in identifying the part of the function proportional to e^{ikr} in the last term in (9.8) with scattered particles?

To answer these questions, we have to consider the motion of wave packets. Take the case of particle transmission through a potential barrier. The potential has the form (Figure 5)

$$\left.\begin{aligned} U &= U_0 \quad \text{for } -a < x < a, \\ U &= 0 \quad \text{for } x < -a,\ a < x. \end{aligned}\right\} \tag{9.9}$$

The wave function, as we know, can be written in the form

$$\psi_E(x, t) = \begin{cases} (e^{ikx} - A(k)\,e^{-ikx})\,e^{-i\frac{Et}{\hbar}} & \text{for } x < -a, \\ B(k)\,e^{ikx - i\frac{Et}{\hbar}} & \text{for } x > a, \end{cases} \tag{9.10}$$

where A is generally called the reflection coefficient.

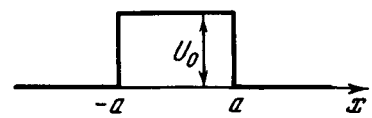

FIGURE 5.

Now we combine states with energy $E \approx E_0$ into a wave packet,

$$\psi(x, t) = \frac{1}{2\Delta E} \int_{E_0-\Delta E}^{E_0+\Delta E} dE \psi_E(x, t), \tag{9.11}$$

where ΔE is assumed to be so small that the energy dependence of A and B is ignorable and for k we use the approximate expression

$$k = k_0 + (E - E_0)\left(\frac{dk}{dE}\right)_0 + \ldots = k_0 + \frac{E - E_0}{\hbar v_0}. \tag{9.12}$$

Elementary calculations give

$$\psi(x, t) = \begin{cases} \varphi^{(+)}(x, t) - A(k_0)\varphi^{(-)}(x,t) & \text{for } x < -a, \\ B(k_0)\varphi^{(+)}(x, t), & \text{for } x > a, \end{cases} \tag{9.13}$$

where

$$\varphi^{(\pm)}(x, t) \equiv \frac{1}{2\Delta E} \int_{E_0-\Delta E}^{E_0+\Delta E} dE e^{i\left(\pm kx - \frac{Et}{\hbar}\right)} = e^{i\left(\pm k_0 x - \frac{E_0 t}{\hbar}\right)} \frac{\sin(x \mp v_0 t)}{(x \mp v_0 t)}.$$

The function $\varphi^{(+)}(x, t)$ does not vanish only when $x - v_0 t \approx 0$, and $\varphi^{(-)}$ does not vanish only for $x + v_0 t \approx 0$. Consider the region to the left of the barrier, where $x < 0$. We see from Figure 6 that for $t < 0$ only $\varphi^{(+)}$ does not vanish (the wave from minus infinity incident on the barrier). For $t > 0$ the position changes: there is no term $\varphi^{(+)}$ left of the barrier, but the term $\varphi^{(-)}$ is no longer zero (a wave reflected from the barrier). To the right of the barrier $x > 0$, and therefore the condition $x - v_0 t = 0$ can be satisfied only for $t > 0$. Thus, for $t < 0$ the wave function is identically zero everywhere to the right of the barrier. For $t > 0$, on the other hand, a wave $B(k_0)\varphi^{(+)}$ is formed, propagating in the direction $x \to +\infty$.

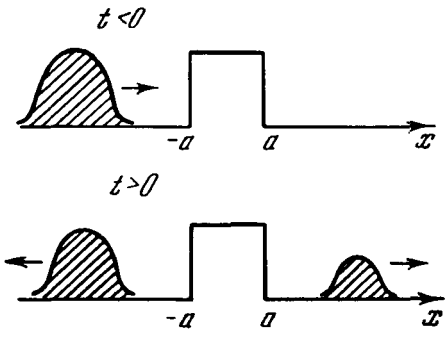

FIGURE 6.

The coefficients $A(k_0)$ and $B(k_0)$ clearly determine the intensities of the reflected and the transmitted wave, and we see that e^{ikx} and e^{-ikx} may indeed be interpreted with complete justification as the wave functions of particles propagating in the directions $x = +\infty$ and $x = -\infty$, respectively.

Let us further consider the normalization of continuum wave functions. The continuum functions $\chi_k(r)$ vanish nowhere in the entire space, and they cannot be normalized to unity as in the case of a discrete spectrum. Normalization to unity corresponds to a condition that there is but a single particle in the entire space. Since a continuum function is everywhere different from zero, normalization to a single particle in the entire space

(i.e., $\int_0^\infty |\chi_k(r)|^2 dr = 1$) is feasible only if we take a zero normalization coefficient $A(k)$. There is, of course an alternative approach, defining normalization in the limit: we first take not the entire space but only the bounded region enclosed in a large sphere of radius R. Here the range $0 < r < R$ is bounded and we can find a finite normalization constant $A(k)$. In the final result R is allowed to go to infinity, and A to zero, so that the product $|A|^2 R$ remains constant. This procedure, however, is unnecessarily complicated, and is hardly ever used.

The common normalization procedure calls for normalization to the δ-function:

$$\int_0^\infty \chi_k(r)\,\chi^*_{k'}(r)\,dr = \delta(k-k'). \tag{9.14}$$

We will now prove the feasibility of this normalization. Consider two close values k and k_1:

$$\chi''_k + (k^2 - V)\chi_k = 0,$$
$$\chi''_{k_1} + (k_1^2 - V)\chi^*_{k_1} = 0.$$

We multiply the first equation by $\chi^*_{k_1}$ and the second by χ_k and then subtract one from the other:

$$\chi^*_{k_1}\chi''_k - \chi_k\chi^{*\prime\prime}_{k_1} = (k_1^2 - k^2)\,\chi_k\chi^*_{k_1}.$$

Integration over r thus gives

$$\int_0^R \chi_k\chi^*_{k_1}\,dr = \frac{1}{k_1^2 - k^2}\left(\chi'_k(r)\,\chi^*_{k_1}(r) - \chi_k(r)\,\chi^{*\prime}_{k_1}(r)\right)\Big|_0^R. \tag{9.15}$$

All the functions vanish at the lower limit; using the asymptotic expression for the wave functions $\chi_k \sim A(k)\sin(kr + \delta)$, we obtain after some manipulations

$$\int_0^R \chi_k\chi^*_{k_1}\,dr = A(k)\,A^*(k_1)\left\{\frac{(k+k_1)\sin[(k_1-k)R + \delta(k_1) - \delta(k)]}{2(k_1^2 - k^2)} - \right.$$
$$\left. - \frac{1}{2(k+k_1)}\sin[(k+k_1)R + \delta(k) + \delta(k_1)]\right\}.$$

Since $R \to \infty$, the last term is effectively equal to zero. Indeed, it is a rapidly oscillating function of k and k_1, and the frequency of oscillations goes to infinity with R. Any integral whose integrand comprises such an oscillating function multiplied by some sufficiently smooth function falls off to zero. It is in this sense that we mean that the functions are effectively equal to zero.

If $(k_1 - k)$ is a fixed finite quantity, the first term is also effectively equal to zero. Let us now consider the case $(k_1 - k) \to 0$. First note that the difference $\delta(k_1) - \delta(k)$ is ignorable compared to $R(k_1 - k)$, so that

$$\int_0^R \chi_k(r)\,\chi^*_{k_1}(r)\,dr = A(k)\,A^*(k_1)\,\frac{1}{2}\,\frac{\sin(k_1-k)R}{(k_1-k)}. \tag{9.16}$$

However, we know that

$$\lim_{a\to\infty} \frac{\sin ax}{x} = \pi\delta(x). \tag{9.17}$$

The graph of $\frac{\sin ax}{x}$ is shown in Figure 7. This function is relatively large for $x \sim \frac{1}{a}$ and rapidly falls off with increasing x. In the limit as $a \to \infty$ this function is zero for $x \neq 0$ and infinity for $x = 0$. The area under the curve is

$$\int_{-\infty}^{\infty} \frac{\sin ax}{x}\, dx = \pi.$$

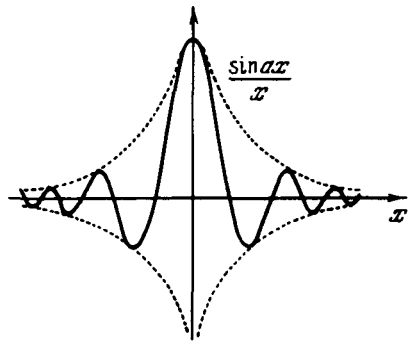

FIGURE 7.

We have thus proved equality (9.17). Using this equality, we write (9.16) in the form

$$\int_0^{\infty} \chi_k(r)\, \chi_{k'}^*(r)\, dr = |A(k)|^2 \frac{\pi}{2} \delta(k - k'). \tag{9.18}$$

The feasibility of δ-function normalization is thus established, and the corresponding normalization coefficient is

$$A(k) = \sqrt{\frac{2}{\pi}}. \tag{9.19}$$

Sometimes the continuum functions are conveniently normalized to $\delta(\varphi(k) - \varphi(k'))$, where $\varphi(k)$ is some function of k. The corresponding normalization constant is

$$A(\varphi(k)) = \sqrt{\frac{dk}{d\varphi(k)}}\, A(k). \tag{9.20}$$

For example, in case of normalization to the energy δ-function $\varphi = \frac{\hbar^2 k^2}{2m}$ and the normalization constant is

$$A(E) = \sqrt{\frac{2}{\pi\hbar v}}. \tag{9.21}$$

Discrete spectrum functions vanish for $r \to \infty$. By (9.15) we therefore immediately have that the continuum functions are orthogonal to all the discrete spectrum functions.* Moreover, any two discrete spectrum functions with different energies $E_m \neq E_n$ are also orthogonal. We may therefore always normalize the wave functions so as to obtain an orthonormal system:

$$\left.\begin{aligned} \int \chi_m(r)\,\chi_n^*(r)\,dr = \delta_{mn}, \quad \int \chi_k(r)\,\chi_{k'}^*(r)\,dr = \delta(k-k'), \\ \int \chi_k(r)\,\chi_n^*(r)\,dr = 0. \end{aligned}\right\} \tag{9.22}$$

Here δ_{mn} is Kronecker's delta.

The wave functions of the continuum and the discrete spectrum constitute a complete system. This means that any sufficiently decent function $f(r)$ can be expanded in functions of this system,

$$f(r) = \int dk C(k)\,\chi_k(r) + \sum_n C_n \chi_n(r). \tag{9.23}$$

The coefficients $C(k)$ and C_n are easily obtained multiplying the two sides of (9.23) by $\chi_k^*(r)$ and $\chi_n^*(r)$ and integrating over r:

$$C(k) = \int \chi_k^*(r')\,f(r')\,dr', \quad C_n = \int \chi_n^*(r')\,f(r')\,dr'. \tag{9.24}$$

Insertion of (9.24) in (9.23) gives

$$f(r) = \int \left[\sum_n \chi_n(r)\,\chi_n^*(r') + \int dk \chi_k(r)\,\chi_k^*(r')\right] f(r')\,dr'. \tag{9.25}$$

Hence it follows that the expression in brackets can be identified with the δ-function:

$$\sum_n \chi_n(r)\,\chi_n^*(r') + \int_0^\infty dk \chi_k(r)\,\chi_k^*(r') = \delta(r-r'). \tag{9.26}$$

If the continuum functions are normalized to the energy δ-function, expressions (9.23)—(9.26) remain valid provided that χ_k is replaced by χ_E and the integrals over k are changed to integration over E.

§ 10. MOTION WITH ORBITAL MOMENTUM $l \neq 0$. MOTION IN A COULOMB FIELD

The wave function of a particle in a state with a given orbital momentum l and given momentum projection m has the form $\frac{\chi_{kl}(r)}{r} Y_{lm}(\theta, \varphi)$, where

$$Y_{lm}(\theta, \varphi) = \frac{1}{\sqrt{2\pi}} \Theta_{lm}(\theta)\, e^{im\varphi},$$

and χ_{kl} is to be found from equation (1.5).

* Note that if the continuum functions are replaced by free motion functions, the latter are no longer orthogonal to the discrete spectrum functions, and this may lead to considerable errors in calculations.

The properties of spherical functions which describe the angular dependence of a wave function with given l and m have been studied in fairly great detail.

We will only consider here a number of theorems which readily follow from the general physical arguments and the analogies derived in the limit of classical motion. *

We start with a function corresponding to maximum $|m|$, i.e., $m = \pm l$. In this case $\Theta_{ll}(\theta)$ clearly has no nodes (since $\sin m\varphi$ and $\cos m\varphi$ have the maximum number of nodes). In the limit of large l this case corresponds to an orbit lying in the equatorial plane with the angular momentum vector along the z-axis. In this limiting case we thus have $|\Theta_{ll}(\theta)|^2 = \delta\left(\theta - \frac{\pi}{2}\right)$.

This estimate can be improved by finding the law according to which $|\Theta_{ll}(\theta)|^2$ approaches $\delta\left(\theta - \frac{\pi}{2}\right)$ with increasing l, growing narrower and concentrating toward the equator.

Note that the square of the angular momentum is $l(l+1)$ and its projection m on the z axis is equal to l. We can thus find the average angle α between the z axis and the normal to the orbital plane, $\cos\alpha = \frac{l}{\sqrt{l(l+1)}} \approx \approx 1 - \frac{1}{2l}$, $\alpha \approx \sqrt{\frac{1}{l}}$. It is readily seen that the average angle β between a vector lying in this inclined plane and the equatorial plane is $\sqrt{\overline{\beta^2}} = \frac{1}{\sqrt{2}}\alpha = \sqrt{\frac{1}{2l}}$.

Thus for large but finite l, $|\Theta_{ll}(\theta)|^2$ has a maximum at $\theta = \frac{\pi}{2}$ and its effective width is $\sqrt{\frac{1}{2l}}$. This means that it can be approximately replaced by $\frac{\sqrt{l}}{\sqrt{\pi}} e^{-l\left(\theta - \frac{\pi}{2}\right)^2}$; the pre-exponential coefficient is determined from the normalization of spherical harmonics.

How are we to envisage the opposite extreme case, namely a function with given large l and with $m = 0$? Such functions are encountered, in particular, in scattering problems, since a particle which moves along the z axis identically has $m = 0$.

The properties of the sought function can be elucidated by considering motion of particles in circular orbits. Take the set of all circular orbits with axes perpendicular to the z axis, i.e., circular orbits in the x, y plane (for these orbits $m = 0$). All the directions in the x, y plane are equiprobable for the orbit axis.

All orbits intersect at the poles and the probability density per surface area of unit solid angle (i.e., per unit surface area of a sphere) is maximum, going to infinity at the poles for $\theta = 0$ and $\theta = \pi$.

We will now derive an expression for this probability density. As one moves along the meridian, all the $d\theta$ intervals are equiprobable, $dW = \frac{d\theta}{\pi}$. Dividing dW by the area which corresponds to the angle $d\theta$, $dS = 2\pi \sin\theta\, d\theta$, we find

$$\overline{|Y_{l0}|^2} = \frac{dW}{dS} = \frac{1}{2\pi^2 \sin\theta}.$$

* A similar treatment of Clebsch—Gordan and Racah coefficients was given by Wigner /74/.

It should be noted that $Y_{l0}(\theta)$ is actually an alternating function with l nodes in the interval $0 \leqslant \theta \leqslant \pi$ (its l node lines are the parallels); the above expression is significant in so far as we ignore these oscillations. The oscillations are ignorable only if $l \gg 1$, and we take $\Delta\theta > \frac{1}{l}$.

Let us estimate the maximum deviation from spherical symmetry for $m = 0$ and $l \gg 1$. We see from the above expression that the density is minimum at the equator: for $\theta = \frac{\pi}{2}$ the average $\overline{|Y_{l0}|^2}$ is equal to $\frac{1}{2\pi^2}$, whereas the average for the entire sphere is $\frac{1}{4\pi}$. The density near the equator is less than the average by a factor of $\frac{\pi}{2}$. Note that, strictly speaking, the density fluctuates from 0 to $\frac{4}{\pi}$ if the fine structure (the nodes) is taken into consideration; for odd l, $\Theta \equiv 0$ on the equator; for even l, $|Y_{l0}|^2 / \frac{1}{4\pi} = \frac{4}{\pi}$, and $\frac{2}{\pi}$ is obtained by averaging over the oscillations. It is remarkable that an asymptotic value independent of l exists in the limit of $l \gg 1$. Near the poles $|Y_{l0}|^2 \to \infty$ when $l \to \infty$. For finite l, the maximum is observed for $\theta = 0$ and $\theta = \pi$:

$$|Y_{l0}(0, \varphi)|^2 = |Y_{l0}(\pi, \varphi)|^2 \approx \frac{l}{2\pi}.$$

If the experimental angular distribution is stretched along the z axis more and near the equator less than by $\frac{2}{\pi} = 0.65$ of the average, we can be certain that we are dealing with interference of states with different l.

Now, asymmetry relative to the equatorial plane, i.e., asymmetry for $z > 0$ and $z < 0$, is clearly possible only in the result of interference between states with even and odd l.

For particles of spin 1/2 the total momentum j is a half-integer. Every j can be formed in two different ways, $j = l_1 + {}^1/_2$ and $j = l_2 - {}^1/_2$.

The wave functions are products of orbit and spin functions, formed in compliance with the rules for momentum composition. We introduce the following notation for spin functions:

$$\alpha \to s_z = \frac{1}{2}, \quad \beta \to s_z = -\frac{1}{2}.$$

Explicit expressions for a few of the first wave functions are given below:

$$\left.\begin{aligned}
&l = 0,\ j = \tfrac{1}{2},\ (S_{1/2}) \\
&\qquad m = \tfrac{1}{2}, \qquad \psi = \frac{1}{\sqrt{4\pi}}\alpha = Y_{0,0}\alpha, \\
&\qquad m = -\tfrac{1}{2}, \qquad \psi = \frac{1}{\sqrt{4\pi}}\beta = Y_{0,0}\beta; \\
&\qquad m = \tfrac{1}{2}, \quad \psi = -\sqrt{\tfrac{1}{3}}Y_{1,0}\alpha + \sqrt{\tfrac{2}{3}}Y_{1,1}\beta, \\
&l = 1,\ j = \tfrac{1}{2},\ (P_{1/2}) \\
&\qquad m = -\tfrac{1}{2}, \quad \psi = -\sqrt{\tfrac{2}{3}}Y_{1,-1}\alpha + \sqrt{\tfrac{1}{3}}Y_{1,0}\beta;
\end{aligned}\right\} \qquad (10.1)$$

$$
\left.
\begin{aligned}
&l=1,\ j=\tfrac{3}{2},(P_{3/2})\\
&\qquad m=\tfrac{3}{2}, \quad \psi=Y_{1,1}\alpha,\\
&\qquad m=\tfrac{1}{2}, \quad \psi=\sqrt{\tfrac{2}{3}}Y_{1,0}\alpha+\sqrt{\tfrac{1}{3}}Y_{1,1}\beta,\\
&\qquad m=-\tfrac{1}{2}, \quad \psi=\sqrt{\tfrac{1}{3}}Y_{1,-1}\alpha+\\
&\qquad\qquad\qquad\qquad +\sqrt{\tfrac{2}{3}}Y_{1,0}\beta,\\
&\qquad m=-\tfrac{3}{2}, \quad \psi=Y_{1,-1}\beta;\\
&l=2,\ j=\tfrac{3}{2},\ (D_{3/2})\\
&\qquad m=\tfrac{3}{2}, \quad \psi=-\sqrt{\tfrac{1}{5}}Y_{2,1}\alpha+\\
&\qquad\qquad\qquad\qquad +\sqrt{\tfrac{4}{5}}Y_{2,2}\beta,\\
&\qquad m=\tfrac{1}{2}, \quad \psi=-\sqrt{\tfrac{2}{5}}Y_{2,0}\alpha+\sqrt{\tfrac{3}{5}}Y_{2,1}\beta,\\
&\qquad m=-\tfrac{1}{2}, \quad \psi=-\sqrt{\tfrac{3}{5}}Y_{2,1}\alpha+\sqrt{\tfrac{2}{5}}Y_{2,0}\beta,\\
&\qquad m=-\tfrac{3}{2}, \quad \psi=-\sqrt{\tfrac{4}{5}}Y_{2,-2}\alpha+\sqrt{\tfrac{1}{5}}Y_{2,-1}\beta.
\end{aligned}
\right\} \qquad (10.1)
$$

A remarkable property of these functions is that the total particle density after averaging over the spin directions depends only on j and m, i.e., it is the same for $j = l_1 + 1/2$ and $j = l_2 - 1/2$. Thus, for example, for $j = \frac{3}{2}$, $m = \frac{3}{2}$ we have in the first case $(P_{3/2})$

$$|\psi|^2 = \frac{1}{4\pi}\frac{3}{2}\sin^2\theta = \frac{1}{4\pi}\left(1-\frac{1}{2}(3\cos^2\theta-1)\right),$$

and in the second case $(D_{3/2})$

$$|\psi|^2 = \frac{1}{4\pi}\left(\frac{3}{2}\cos^2\theta\sin^2\theta+\frac{3}{2}\sin^4\theta\right) = \frac{1}{4\pi}\left(1-\frac{1}{2}(3\cos^2\theta-1)\right),$$

i.e., both results are equal.

In the particular case $j = \frac{1}{2}$ the total density is isotropic not only for $S_{1/2}$ $(l = 0)$ but also for $P_{1/2}$ $(l = 1)$:

$$|\psi_{S_{1/2}}|^2 = |\psi_{P_{1/2}}|^2 = \frac{1}{4\pi}.$$

We can distinguish between $l_1 + \frac{1}{2}$ and $l_2 - \frac{1}{2}$ only by polarization measurements, i.e., by measuring both the total particle density and the spin direction.

Interference between $l_1 + \frac{1}{2}$ and $l_2 - \frac{1}{2}$ creates asymmetry of total density about the equator. In particular, although the individual states $S_{1/2}$ and $P_{1/2}$ are isotropic, interference of these states produces anisotropy: the maximum corresponds to the linear combination

$$\psi = \frac{1}{\sqrt{2}} [\psi_{S_{1/2}} \pm \psi_{P_{1/2}}].$$

In this case $W = |\psi|^2 = \frac{1}{4\pi} (1 \mp \cos\theta)$.

The above properties are specific of spin 1/2 particles, and it is these particles which are of the greatest importance in practical considerations.

We will now proceed with a discussion of radial wave functions.

Virtually all the specific nuclear interactions are short-range interactions, i.e., they can be taken equal to zero outside a certain sphere $r = R$. The centrifugal potential which enters the Sch. Eq. for $l \neq 0$, on the other hand, extends far beyond any sphere $r=R$ and essentially modifies the form of the wave function for $r > R$.

For $r > R$, the equation for χ_{kl} has the form

$$\chi''_{kl} + \left(k^2 - \frac{l(l+1)}{r^2}\right) \chi_{kl} = 0,$$

which is reduced to Bessel's equation by a substitution $\chi = \sqrt{r} Z$. The general solution of this equation in the exterior region is thus

$$\chi_{kl}(r) = \sqrt{r}\, Z_{l+1/2}(kr),$$

where $Z_{l+1/2}$ is any of Bessel's functions of order $l + 1/2$.

As the two independent solutions we choose

$$\left.\begin{aligned} \chi^{(+)}_{kl}(r) &= i \sqrt{\frac{\pi kr}{2}} H^{(1)}_{l+1/2}(kr) \equiv (kr)\, h^{(1)}_l(kr), \\ \chi^{(-)}_{kl}(r) &= -i \sqrt{\frac{\pi kr}{2}} H^{(2)}_{l+1/2}(kr) \equiv (kr)\, h^{(2)}_l(kr), \end{aligned}\right\} \tag{10.2}$$

where $H^{(1)}$ and $H^{(2)}$ are Hankel's functions.* For large kr these two solutions behave as

$$\chi^{(\pm)}_{kl}(r) \sim e^{\pm i\left(kr - \frac{l\pi}{2}\right)} \tag{10.3}$$

and correspond to incoming and outgoing particle fluxes. These solutions are a generalization for $l \neq 0$ of the functions $\chi^{(\pm)}_{k0}$ and have the same physical interpretation. The continuum functions describing the scattering of a particle of momentum l can be written by analogy with (9.6) and (9.8) in the form

$$\left.\begin{aligned} \chi_{kl} &= A_l(k) \left(\chi^{(-)}_{kl} - S_l(k)\, \chi^{(+)}_{kl}\right), \\ \chi_{kl} &\sim -2iA_l(k)\, e^{i\delta_l} \sin\left(kr - \frac{\pi l}{2} + \delta_l\right) \text{ for } r \to \infty. \end{aligned}\right\} \tag{10.4}$$

* These functions are polynomials of degree l of the argument $\frac{1}{kr}$, multiplied by $e^{\pm i\left(kr - \frac{\pi l}{2}\right)}$. Their explicit form is obtained from the formula

$$\chi^{(\pm)}_{kl}(r) = (-1)^l (kr)^{l+1} \left(\frac{d}{k^2 r\, dr}\right)^l \frac{e^{\pm ikr}}{kr}.$$

Here $e^{2i\delta_l} \equiv S_l(k)$ has the same role as S_0 for $l = 0$. If the potential U is identically zero, the above expression for the wave function should be valid in the entire space. The functions $\chi_{kl}^{(\pm)}$, however, behave for small kr as

$$\chi_{kl}^{(\pm)} \sim \frac{\Gamma\left(l+\frac{1}{2}\right)}{\sqrt{\pi}} \left(\frac{2}{kr}\right)^l, \tag{10.5}$$

(here Γ is the gamma function) and are clearly irregular at the origin. To obtain a regular function, we should form the difference

$$\frac{1}{2i}\left(\chi_{kl}^{(+)} - \chi_{kl}^{(-)}\right) \equiv \sqrt{\frac{\pi kr}{2}} J_{l+\frac{1}{2}}(kr) \sim \frac{\sqrt{\pi}}{\Gamma\left(l+\frac{3}{2}\right)} \left(\frac{kr}{2}\right)^{l+1}, \tag{10.6}$$

where

$$J_{l+\frac{1}{2}}(kr) \equiv \frac{1}{2}\left(H_{l+\frac{1}{2}}^{(1)}(kr) - H_{l+\frac{1}{2}}^{(2)}(kr)\right)$$

is the ordinary Bessel function, and this difference vanishes at the origin. *

Comparison of (10.4) with (10.6) shows that in case of zero potential the phase δ_l vanishes and $S_l(k) = 1$, in complete analogy with the results of § 9. The scattering power of the potential is determined, as before, by $|S_l(k) - 1|^2$. As regards $S_l(k)$ itself, it cannot be computed unless the solution $\chi_{kl}^{(0)}(r)$ of the Sch. Eq. inside the potential range ($r < R$) has been found. As soon as this solution is known, $S_l(k)$ is calculated by (1.11), where $\chi_k^{(\pm)}$ and $\chi_k^{(0)}$ are replaced by their analogs $\chi_{kl}^{(\pm)}$ and $\chi_{kl}^{(0)}$. It is also easily seen that expressions (9.18) – (9.26), which define the normalization for $l = 0$, remain valid for χ_{kl} with any l.

We thus see that the case $l \neq 0$ differs from that of § 9 ($l = 0$) only quantitatively but not qualitatively. The physical interpretation and the qualitative features of the solutions of the Sch. Eq. are the same in both cases.

We have so far worked with a neutral, uncharged particle. Let us now consider the case of Coulomb forces acting on the particle in addition to the potential $U(r)$. The charge of the particle is e_1, and the charge at the point $r = 0$ is e_2.

The total potential seen by the particle is now given by

$$\left.\begin{aligned} V(r) + \frac{l(l+1)}{r^2} + \frac{2\eta k}{r} \text{ for } r < R, \\ \frac{l(l+1)}{r^2} + \frac{2\eta k}{r} \text{ for } r > R, \end{aligned}\right\} \tag{10.7}$$

where $\eta = \frac{e_1 e_2}{\hbar v}$, v is the velocity of the particle.

For $r > R$, the Sch. Eq. has the form

$$\chi_{kl}'' + \left(k^2 - \frac{l(l+1)}{r^2} - \frac{2\eta k}{r}\right)\chi_{kl} = 0. \tag{10.8}$$

The properties of this equation have been studied in considerable detail. Its two independent solutions are generally chosen as the so-called regular

* This behavior of the wave function for small r is easily elucidated from equation (1.5).

and irregular Coulomb functions $F_l(kr, \eta)$ and $G_l(kr, \eta)$. For $r \to \infty$ these functions give

$$\left.\begin{aligned} F_l &\sim \sin\left\{kr - \frac{l\pi}{2} + \eta_l - \eta \ln 2kr\right\}, \\ G_l &\sim \cos\left\{kr - \frac{l\pi}{2} + \eta_l - \eta \ln 2kr\right\}, \end{aligned}\right\} \tag{10.9}$$

where $\eta_l = \arg\Gamma(l + 1 + i\eta)$. For $r \to 0$, F_l approaches zero as r^{l+1}, and G_l goes to infinity as r^{-l}:

$$\left.\begin{aligned} F_l(kr, \eta) &\underset{r\to 0}{\sim} C_l (kr)^{l+1}, \\ G_l(kr, \eta) &\underset{r\to 0}{\sim} \frac{1}{(2l+1)C_l}(kr)^{-l}, \end{aligned}\right\} \tag{10.9'}$$

where

$$C_l = \frac{2^l}{(2l+1)!}\left[(1^2+\eta^2)(2^2+\eta^2)\ldots(l^2+\eta^2)\right]^{1/2} C_0,$$
$$C_0 = \left[\frac{2\pi\eta e^{-2\pi\eta}}{1-e^{-2\pi\eta}}\right]^{1/2}.$$

In the following, we will use linear combinations of the Coulomb functions:

$$\chi_{kl}^{(\pm)}(r) = G_l \pm iF_l \sim e^{\pm i\left(kr - \frac{l\pi}{2} + \eta_l - \eta \ln 2kr\right)}. \tag{10.9''}$$

These functions, by analogy with the functions (10.3) defined in the preceding, describe outgoing and incoming particle fluxes (v particles through a sphere of large radius every second). This is easily verified if we compute the corresponding fluxes. The term with ln $2kr$ in the exponential can be treated as constant, since on differentiation with respect to r it gives a contribution which vanishes for $r \to \infty$ faster by a factor of r than the principal term.

For positive energies, the general solution of the Sch. Eq. in the region $r > R$ can be written by analogy with the previous treatment in the form

$$\begin{aligned} \chi_{kl}(r) &= A_l(k)\left(\chi_{kl}^{(-)}(r) - S_l \chi_{kl}^{(+)}(r)\right) \sim \\ &\sim -2iA_l(k)\, e^{i\delta_l} \sin\left(kr - \frac{\pi l}{2} + \eta_l + \delta_l - \eta \ln 2kr\right), \\ S_l(k) &\equiv e^{2i\delta_l}. \end{aligned} \tag{10.10}$$

If the potential $U(r)$ identically vanishes, the solution (10.10) should hold true in the entire space. In this case $S_l \equiv 1$ and $\delta_l = 0$. Indeed, we know that only one of the Coulomb functions, F_l, is regular at the origin. This means that (10.10) should not contain G_l, i.e., $S_l = 1$.

For nonzero $U(r)$, we have $S_l \neq 1$ and δ_l is a characteristic of the scattering power of the potential $U(r)$. χ_{kl} is conveniently written with the pure "Coulomb" part separated:

$$\begin{aligned} \chi_{kl}(r) &= A_l(k)\left\{\chi_{kl}^{(-)} - \chi_{kl}^{(+)} - (S_l - 1)\chi_{kl}^{(+)}\right\} = \\ &= A_l(k)\left\{-2iF_l - (S_l - 1)\chi_{kl}^{(+)}\right\}. \end{aligned} \tag{10.11}$$

The last term in this expression is entirely attributable to scattering by the potential $U(r)$ and it vanishes when the potential is zero.

§ 11. CONTINUUM WAVE FUNCTIONS. SCATTERING CROSS SECTION (NEUTRAL PARTICLES)

We have so far dealt only with particles with a definite angular momentum relative to the origin. In scattering problems, however, we are dealing with a beam of particles propagating with a definite velocity in a definite direction in a scattering field $U(r)$. The way to approach this problem is the following.*

A linear beam of particles moving in the direction $\boldsymbol{k}$ is described by a plane wave $e^{i\boldsymbol{kr}}$ Indeed, the current corresponding to a plane wave is

$$j = \frac{\hbar \boldsymbol{k}}{m} = \boldsymbol{v}.$$

The angular momentum of these particles relative to the origin is undefined, since the probability density $|e^{i\boldsymbol{kr}}|^2 = 1$ is constant throughout the space and in classical terms any values of the impact parameter are permissible for a given velocity. The fraction of states with different angular momenta l relative to the origin can be found from the expansion of a plane wave in spherical harmonics:

$$e^{i\boldsymbol{kr}} = \sum_{l=0}^{\infty} i^l (2l+1) P_l\left(\frac{\boldsymbol{kr}}{kr}\right) j_l(kr) =$$
$$= \frac{1}{ikr} \sum i^l \sqrt{\pi (2l+1)}\, Y_{l0}\left(\frac{\boldsymbol{kr}}{kr}\right) (\chi_{kl}^{(+)}(r) - \chi_{kl}^{(-)}(r)). \tag{11.1}$$

Here P_l are the Legendre polynomials, Y_{l0} are the spherical harmonics, and $\chi_{kl}^{(\pm)}$ are defined by (10.2). We see from this expansion that the incoming wave $\frac{\chi_{kl}^{(-)}}{r}\, Y_{l0}$ with momentum l is contained in the plane wave with the amplitude

$$C_l = -\frac{1}{ik}\, i^l \sqrt{\pi (2l+1)}. \tag{11.2}$$

In classical physics the angular momentum of a particle relative to some point $r = 0$ is $\boldsymbol{L} = [\boldsymbol{rp}]$, and its projection on the direction of motion is zero. This theorem is valid in quantum mechanics also: the function $Y_{lm}(\theta, \varphi)$ corresponds to a state with angular momentum l and projection m on the quantization axis (i.e., on the direction of particle motion in the particular frame). That $e^{i\boldsymbol{kr}}$ is expanded only in terms of Y_{l0} actually signifies that the particle beam moving in the direction of $\boldsymbol{k}$ contains various angular momenta l relative to the point $r = 0$, but the projection of the angular momentum on the direction $\boldsymbol{k}$ is invariably zero.

Expression (11.2) implies that the wave function describing scattering of a linear beam should have the form

$$\psi_{\boldsymbol{k}}(\boldsymbol{r}) = \sum C_l Y_{l0}\left(\frac{\boldsymbol{kr}}{kr}\right) \frac{1}{r} (\chi_{kl}^{(-)} - S_l \chi_{kl}^{(+)}). \tag{11.3}$$

* The general method of solution presented in this section was first applied by Faxen and Holtsmark /75/; a particular case of scattering of sound waves by an impenetrable sphere was treated by an analogous method by Rayleigh /76/.

Indeed, waves incident on the force center (i.e., the terms with $\chi^{(-)}$) clearly have the same amplitude as the wave propagating in free space; the amplitudes of the outgoing waves (i.e., the coefficients of $\chi^{(+)}$), however, acquire an additional phase factor $S_l = e^{2i\delta_l}$ due to the effect of the potential $U(r)$.

Expression (11.3) for ψ_k is conveniently written with the scattered wave separated:

$$\psi_k(r) = e^{ikr} + \sum_l C_l Y_{l0}\left(\frac{kr}{kr}\right)(1 - S_l)\frac{1}{r}\chi_{kl}^{(+)} \sim e^{ikr} + f(\theta)\frac{e^{ikr}}{r}; \qquad (11.4)$$

here $f(\theta)$ is the so-called scattering amplitude,

$$f(\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}\sqrt{4\pi(2l+1)}\,Y_{l0}\left(\frac{kr}{kr}\right)(S_l - 1),\ \cos\theta = \frac{kr}{kr}. \qquad (11.5)$$

If the potential $U(r)$ is identically zero, all S_l are unity, $f(\theta) = 0$, and no scattering is observed. If the potential does not vanish, $f(\theta) \neq 0$.

Let us calculate the current of particles scattered at an angle θ and emerging from a large sphere through a surface element $r^2 \sin\theta\, d\theta\, d\varphi = r^2\, d\Omega$. The scattered particles are described by the term $f(\theta)\frac{e^{ikr}}{r}$. The corresponding particle flux is

$$j(\theta)\, d\Omega = v|f(\theta)|^2 d\Omega.$$

The so-called scattering cross section $\sigma(\theta)$ is introduced as a characteristic of the scattering power of the potential. It is defined as the flux of scattered particles within a solid angle $d\Omega$ produced by unit flux j (1 particle/cm^2·sec) incident on the force center. The incident current is equal to v. The scattering cross section in a potential $U(r)$ is thus given by

$$\sigma(\theta)\, d\Omega = |f(\theta)|^2 d\Omega. \qquad (11.6)$$

Integration over all the angles gives the total scattering cross section*

$$\sigma = \int \sigma(\theta)\, d\Omega = \frac{\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)|S_l - 1|^2 = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l, \qquad (11.7)$$

which is a sum of cross sections for states with different l:

$$\sigma = \sum_l \sigma_l, \quad \sigma_l \equiv \frac{\pi(2l+1)}{k^2}|S_l - 1|^2. \qquad (11.8)$$

The scattering cross section at a given angle $\sigma(\theta)$ (the so-called differential cross section) cannot be presented in a similarly simple form. By (11.5) and (11.6) $\sigma(\theta)$ is written as

$$\sigma(\theta) = \frac{\pi}{k^2}\sum_{l,l_1}\sqrt{(2l+1)(2l_1+1)}\,Y_{l0}Y_{l_1 0}^{*}(S_l - 1)(S_{l_1}^{*} - 1),$$

* In classical mechanics $\sigma = \infty$ if the potential $U(r)$ does not vanish for r greater than some R. A remarkable feature of quantum mechanics is that the cross section is finite for all potentials falling off faster than $1/r$. An essential difference between the classical and the quantum cross sections clearly becomes apparent for small-angle scattering.

so that it contains interference terms $Y_{l0}Y^*_{l,0}$ between states with different orbital momenta l. The interference terms cancel out only when we integrate over all the angles, as the spherical harmonics are orthogonal.

The functions $\psi_k(r)$ can be written in a very illustrative form. We use the following equality

$$\frac{1}{2}\sum_{l=0}^{\infty}(2l+1)P_l(\boldsymbol{nn}_1) \equiv \sum_{l=0}^{\infty}\sqrt{\pi(2l+1)}\,Y_{l0}(\boldsymbol{nn}_1) = \\ = 2\pi\delta(1-\boldsymbol{nn}_1) = 2\pi\delta(\boldsymbol{n}-\boldsymbol{n}_1), \tag{11.9}$$

where $\boldsymbol{n}$ and $\boldsymbol{n}_1$ are any two unit vectors, and $\delta(\boldsymbol{n}-\boldsymbol{n}_1)$ is the δ-function. Equality (11.9) is readily verified by multiplying both sides by $Y_{l,0}(\boldsymbol{nn}_1)$ and integrating over all the directions of one of the two vectors, say $\boldsymbol{n}$: $d\boldsymbol{n} = \sin\theta\, d\theta\, d\varphi$.

From (11.1) and (11.4), making use of (11.9) and the known relation $Y_{l0}(-\boldsymbol{nn}_1) = (-1)^l Y_{l0}(\boldsymbol{nn}_1)$, we immediately obtain for large r

$$\psi_k(r) \underset{r\to\infty}{\sim} e^{ikr} + f(\theta)\frac{e^{ikr}}{r} = \frac{2\pi}{ikr}\left\{-\delta(\boldsymbol{n}+\boldsymbol{n}_1)e^{-ikr} + \right. \\ \left. + \left[\delta(\boldsymbol{n}-\boldsymbol{n}_1) + \frac{ik}{2\pi}f(\boldsymbol{nn}_1)\right]e^{ikr}\right\}. \tag{11.10}$$

Here $\boldsymbol{n} = \frac{\boldsymbol{k}}{k}$; $\boldsymbol{n}_1 = \frac{\boldsymbol{r}}{r}$.

Expression (11.10) has an obvious meaning: the incoming particle beam has nonzero amplitude only for $\boldsymbol{n}_1 = -\boldsymbol{n}$, which corresponds to particles moving in the direction $\boldsymbol{k}$ toward the origin. The amplitude of the outgoing particles is divided into two parts: unscattered particles which move away from the origin in the direction $\boldsymbol{n}$, and particles scattered in all directions which are described by the term $\frac{ik}{2\pi}f(\boldsymbol{nn}_1)$.

We can now construct a complete orthonormal system of wave functions. To this end, we have to compute the integral

$$\int\psi_k(\boldsymbol{r})\,\psi_{k_1}(\boldsymbol{r})\,d\boldsymbol{r} = (2\pi)^3\sum_{ll_1}\frac{i^{l-l_1}}{16\pi^3 kk_1}4\pi\sqrt{(2l+1)(2l_1+1)}\times \\ \times e^{i(\delta_l(k)-\delta_{l_1}(k))}\int_0^{\infty}\chi_{kl}(r)\,\chi^*_{k_1l_1}(r)\,dr\int d\Omega_r Y_{l0}\left(\frac{\boldsymbol{kr}}{kr}\right)Y^*_{l_1,0}\left(\frac{\boldsymbol{k}_1\boldsymbol{r}}{k_1r}\right).$$

Integration over the angles is elementary:

$$\int d\Omega_r Y_{l0}\left(\frac{\boldsymbol{kr}}{kr}\right)Y^*_{l_1,0}\left(\frac{\boldsymbol{k}_1\boldsymbol{r}}{k_1r}\right) = \delta_{ll_1}\sqrt{\frac{4\pi}{2l+1}}\,Y_{l0}\left(\frac{\boldsymbol{kk}_1}{kk_1}\right).$$

Since the radial functions are normalized to $\delta(k-k_1)$, we obtain

$$\int d\boldsymbol{r}\,\psi_k\psi^*_{k_1} = (2\pi)^2\frac{\delta(k-k_1)}{k^2}\sum_l\sqrt{\pi(2l+1)}\,Y_{l0}\left(\frac{\boldsymbol{kk}_1}{kk_1}\right) = (2\pi)^3\delta(\boldsymbol{k}-\boldsymbol{k}_1). \tag{11.11}$$

Thus, the set of functions $\psi^{(+)}_{\boldsymbol{k}} = \frac{1}{(2\pi)^{3/2}}\psi_{\boldsymbol{k}}$ for all possible vectors $\boldsymbol{k}$ constitute an orthonormal system. However, this system, in general, is not complete.

Indeed, besides the continuum states, we may have the additional solutions

$$\psi_{nlm}(\boldsymbol{r}) = \frac{1}{r}\chi_{nl}(r)\,Y_{lm}(\theta, \varphi),$$
$$\int \psi_{nlm}(\boldsymbol{r})\,\psi^{*}_{n_1l_1m_1}(\boldsymbol{r})\,d\boldsymbol{r} = \delta_{nn_1}\delta_{ll_1}\delta_{mm_1},$$

for some discrete negative energy values E_{nl} (or for the corresponding imaginary wave vectors $k_{nl} = i\varkappa_{nl}$); these solutions describe bound states of a particle with orbital momentum l and projection m in the potential $U(r)$. Moreover, we know from the previous section that the continuum and the discrete-spectrum functions are mutually orthogonal $\int \psi_{nlm}(\boldsymbol{r})\,\psi^{*}_{\boldsymbol{k}}(\boldsymbol{r})d\boldsymbol{r} = 0$. We also know that the functions

$$\psi_{nlm}(\boldsymbol{r}) \quad \text{and} \quad \psi^{(+)}_{\boldsymbol{k}}(\boldsymbol{r}) \tag{11.12}$$

constitute a complete set of Sch. Eq. functions which satisfy the conditions of boundedness and continuity in the entire space. These functions are orthonormal, so that

$$\left.\begin{aligned} \int d\boldsymbol{r}\,\psi_{nlm}(\boldsymbol{r})\,\psi^{*}_{n_1l_1m_1}(\boldsymbol{r})\,d\boldsymbol{r} &= \delta_{nn_1}\delta_{ll_1}\delta_{mm_1}, \\ \int d\boldsymbol{r}\,\psi_{nlm}(\boldsymbol{r})\,\psi^{(+)*}_{\boldsymbol{k}}(\boldsymbol{r}) &= 0, \\ \int d\boldsymbol{r}\,\psi^{(+)}_{\boldsymbol{k}}(\boldsymbol{r})\,\psi^{(+)*}_{\boldsymbol{k}_1}(\boldsymbol{r}) &= \delta(\boldsymbol{k}-\boldsymbol{k}_1). \end{aligned}\right\} \tag{11.13}$$

Since the system is complete, any square-integrable function $\varphi(\boldsymbol{r})$ (i.e., a function for which the integral over the square of the modulus is bounded) can be expanded in these functions:

$$\varphi(\boldsymbol{r}) = \sum_{nlm} C_{nlm}\psi_{nlm}(\boldsymbol{r}) + \int d\boldsymbol{k}\,C(\boldsymbol{k})\,\psi^{(+)}_{\boldsymbol{k}}(\boldsymbol{r}), \tag{11.14}$$

whence, multiplying by $\psi^{*}_{nlm}(\boldsymbol{r})$ or $\psi^{(+)*}_{\boldsymbol{k}_1}(\boldsymbol{r})$ and integrating over $\boldsymbol{r}$, we readily get

$$\left.\begin{aligned} C_{nlm} &= \int d\boldsymbol{r}\varphi(\boldsymbol{r})\psi^{*}_{nlm}(\boldsymbol{r}), \\ C(\boldsymbol{k}) &= \int d\boldsymbol{r}\varphi(\boldsymbol{r})\psi^{(+)*}_{\boldsymbol{k}}(\boldsymbol{r}). \end{aligned}\right\} \tag{11.15}$$

It is obvious that a complete system of functions can be selected in an infinite number of ways. Indeed, as a complete system we may choose, say, the functions

$$\psi_{nlm}(\boldsymbol{r}) \quad \text{and} \quad \psi_{klm}(\boldsymbol{r}) = \frac{1}{r}\chi_{kl}(r)\,Y_{lm}\left(\frac{\boldsymbol{r}}{r}\right), \tag{11.16}$$

or any linear combinations of these functions. The previously introduced functions $\psi^{(+)}_{\boldsymbol{k}}(\boldsymbol{r})$ are indeed one of such combinations of $\psi_{klm}(\boldsymbol{r})$.

In addition to $\psi^{(+)}_{\boldsymbol{k}}$ we sometimes use the functions

$$\psi^{(-)}_{\boldsymbol{k}}(\boldsymbol{r}) \equiv \psi^{(+)*}_{-\boldsymbol{k}}(\boldsymbol{r}). \tag{11.17}$$

These functions have the form

$$\psi_{\mathbf{k}}^{(-)} = \frac{1}{4\pi k} \sum i^l \sqrt{4\pi(2l+1)}\, Y_{l0}\left(\frac{\mathbf{kr}}{kr}\right) e^{-i\delta_l(k)} \frac{1}{r} \chi_{kl}(r). \tag{11.18}$$

Their physical meaning is clearly understood from the asymptotic expression

$$\psi_{\mathbf{k}}^{(-)}(\mathbf{r}) \sim \frac{1}{(2\pi)^{3/2}} \left[e^{i\mathbf{kr}} + f^*\left(-\frac{\mathbf{kr}}{kr}\right) \frac{e^{-ikr}}{r} \right] \sim$$

$$\sim \frac{1}{(2\pi)^{3/2}} \frac{2\pi}{ikr} \left\{ -\left[\delta(\mathbf{n}+\mathbf{n}_1) - \frac{ik}{2\pi} f^*(-\mathbf{n}\mathbf{n}_1) \right] e^{-ikr} + \delta(\mathbf{n}-\mathbf{n}_1) e^{ikr} \right\} \text{ for } r \to \infty. \tag{11.19}$$

We see that although the particles converge to the force center from all directions, the phase relations between the amplitudes of the incident waves with different l are such that the scattered particles emerge only in the direction $\mathbf{k}$; scattering thus converts a convergent incoming beam into a unidirectional beam. *

Taking the complex conjugate of the formulas in the first half of this section and changing the sign of $\mathbf{k}$, we readily see that the functions

$$\psi_{nlm}(\mathbf{r}) \text{ and } \psi_{\mathbf{k}}^{(-)}(\mathbf{r}) \tag{11.20}$$

are orthonormal and constitute a complete set of solutions of the Sch. Eq. (1.2').

The very interpretation of the functions $\psi_{\mathbf{k}}^{(+)}$ and $\psi_{\mathbf{k}}^{(-)}$ gives a clue as to when to prefer the system (11.12), when (11.16), and when (11.20). A state $\varphi(\mathbf{r})$ should be expanded in eigenfunctions (11.12) if we are interested in the distribution (energy and direction) of the incident particles which correspond to the state $\varphi(\mathbf{r})$. If we are interested in the distribution of particles over states with given l, m, and k, we should use (11.16). Finally, if we want to find the distribution of directions and intensities for the outgoing particles, system (11.20) is the best.

Suppose that a state $\varphi(\mathbf{r})$ has been created in some way in the potential $U(r)$, and we inquire as to the number of particles with wave vector $\mathbf{k}$ emerging from the origin. This number is clearly determined by the square of the modulus of the corresponding coefficient

$$C^{(-)}(\mathbf{k}) = \int d\mathbf{r} \varphi(\mathbf{r}) \psi_{\mathbf{k}}^{(-)*}(\mathbf{r}),$$

if we use an expansion in eigenfunctions (11.20). $C^{(-)}(\mathbf{k})$ can also be determined from an expansion in eigenfunctions (11.12), but the procedure would be more lengthy: first we have to expand $\varphi(\mathbf{r})$ in $\psi_{\mathbf{k}_1}^{(+)}$ and find the coefficients

$$C^{(+)}(\mathbf{k}_1) = \int d\mathbf{r} \varphi(\mathbf{r}) \psi_{\mathbf{k}_1}^{(+)*}(\mathbf{r}),$$

* Note that the states $\psi_{\mathbf{k}}^{(+)}$ and $\psi_{\mathbf{k}}^{(-)}$ (often called the in and out states, respectively) reduce to the eigenfunctions of the free Hamiltonian $H_0 = \frac{p^2}{2m}$ for $r \to \infty$. Thus, in our case the total Hamiltonian H is naturally split into H_0 and V. Scattering theory can be developed, however, without dividing the Hamiltonian into these two parts /77/. A rigorous theory of scattering is presented in /78/.

and then compute $C^{(-)}(k)$ from the resulting expansion:

$$C^{(-)}(k) = \int dr \left\{ \int dk_1 C^{(+)}(k_1) \psi_{k_1}^{(+)}(r) \right\} \psi_k^{(-)*}(r).$$

In principle, this technique is in no way inferior to the previous one, but technically it is incomparably and unjustifiably more complicated.

We give one last formula which is a consequence of the completeness property of the eigenfunctions of the Sch. Eq.:

$$\sum_{nlm} \psi_{nlm}(r) \psi_{nlm}^*(r_1) + \int dk \psi_k^{(\pm)}(r) \psi_k^{(\pm)*}(r_1) = \delta(r - r_1). \tag{11.21}$$

§ 12. THE OPTICAL THEOREM AND ITS GENERALIZATION

As we have shown in the previous section, scattering of a particle in a potential field is described by a wave function

$$\psi_k(r) \underset{r\to\infty}{\sim} e^{ikr} + f(n, n') e^{ikr}/r, \quad \text{where } n = k/k, \; n' = r/r.$$

The first term of this function describes the transmitted wave, and the second term is the scattered wave. Therefore, at a first glance, this expression seems to involve a paradox: the beam of particles passes by unimpeded and a certain additional beam is scattered. The scattered beam is thus created from nothing. How are we to reconciliate this apparent paradox with particle number conservation or, equivalently, with probability conservation (i.e., unitarity)? A correct answer to this problem is to be sought in the interference between the incident wave and the wave scattered at an angle 0. This interference depletes the transmitted beam. To obtain a clearer understanding of the mechanism of scattering, let us calculate the current $j(r)$ corresponding to this wave function for $r \to \infty$. Retaining only the slowest terms, we obtain

$$\hat{p}\psi_k = -i\hbar\nabla\psi_k = \hbar k n e^{ikr} + \hbar k n' \frac{f}{r} e^{ikr}. \tag{12.1}$$

Inserting this relation in expression (9.1) for the current, we get

$$\frac{m}{\hbar} j = kn + \frac{1}{2}\frac{k}{r}(n + n')\left[f e^{-i(kr-kr)} + f^* e^{i(kr-kr)} \right] + kn' \frac{|f|^2}{r^2}. \tag{12.2}$$

Finally, using the identity

$$\lim_{r\to\infty} e^{ikrn'r} = \frac{2\pi i}{k}\left[\delta(n + n') \frac{e^{-ikr}}{r} - \delta(n - n') \frac{e^{ikr}}{r} \right], \tag{12.3}$$

we find

$$\frac{m}{\hbar} j = kn - kn \frac{4\pi}{k} \operatorname{Im} f(n', n) \frac{\delta(n - n')}{r^2} + kn' \frac{|f(nn')|^2}{r^2}. \tag{12.4}$$

All the three terms in (12.4) have simple physical meaning: the first term describes the flux of incident particles; the second term, associated with the interference of incident and scattered waves, reduces the particle flux in the primary direction, i.e., causes beam attenuation by scattering; finally the last term is simply the scattered beam.

We now integrate the two sides of (12.4) over a large sphere of radius $r = R$ and transform the surface integral in the left-hand side to an integral over the volume V enclosed within the sphere S:

$$\int_S \boldsymbol{j}\,d\boldsymbol{S} = \int_V \operatorname{div}\boldsymbol{j}\,d\boldsymbol{r}. \tag{12.5}$$

In stationary states div $\boldsymbol{j} = 0$, which follows, e.g., from the continuity equation $\operatorname{div}\boldsymbol{j} + \frac{\partial \rho}{\partial t} = 0$, since $\frac{\partial \rho}{\partial t} = 0$. Expression (12.5) thus takes the form

$$0 = 0 - \frac{4\pi}{k}\operatorname{Im} f(\boldsymbol{n}, \boldsymbol{n}) + \int |f(\boldsymbol{n}, \boldsymbol{n}')|^2\,d\boldsymbol{n}'. \tag{12.6}$$

The last term in (12.6) is the scattering cross section σ, so that

$$\operatorname{Im} f(\boldsymbol{n}, \boldsymbol{n}) = \frac{k}{4\pi}\sigma. \tag{12.7}$$

We have derived the so-called "optical theorem", originally established by Feenberg /79/. This important theorem relates the total cross section to the imaginary part of the forward scattering amplitude. As we have seen, the left-hand side of (12.7) is the result of interference between the amplitudes of unscattered particles and particles scattered at an angle $\theta = 0$ to the incident beam. In other words, the "optical theorem" is a quantum-mechanical effect associated with the wave properties of particle motion.

The above analysis is equally applicable to the functions $\psi_k(\boldsymbol{r})$ and to any linear combination

$$\psi(\boldsymbol{r}) = \int A(\boldsymbol{n})\,\psi_{k\boldsymbol{n}}(\boldsymbol{r})\,d\boldsymbol{n}. \tag{12.8}$$

In this case, the requirement that the integral over the flux should vanish for any $A(\boldsymbol{n})$ leads to the following generalization of the optical theorem:

$$\operatorname{Im} f(\boldsymbol{n}, \boldsymbol{n}') = \frac{k}{4\pi}\int d\boldsymbol{n}''\,f(\boldsymbol{n}, \boldsymbol{n}'')\,f^*(\boldsymbol{n}', \boldsymbol{n}''). \tag{12.9}$$

The reader will easily verify this identity.

Let us now consider another, more ingenious generalization of the "optical theorem" recently proposed by Lippmann /80/.

This generalized "optical theorem" is applicable not only to the scattering of a single particle by a potential but also in a number of other cases. We will therefore proceed with general treatment. Let the Hamiltonian be $H = H_0 + H_1$, where H_1 is responsible for scattering. The wave function $\psi^{(+)}$, analogous to the previous $\psi^{(+)}$ and satisfying the Sch. Eq. $(E - H_0)\psi^{(+)} = H_1\psi^{(+)}$, has the form

$$\psi^{(+)} = \Phi + \frac{1}{E - H_0 + i\varepsilon}H_1\psi^{(+)}, \tag{12.10}$$

where the function Φ is the solution of the equation $H_0\Phi = E\Phi$ and is the analog of the incident wave; the functions Φ constitute a complete system /81/.

Consider any operator A which commutes with H_0. Let Φ_a be an eigenfunction of this operator, $A\Phi_a = A_a\Phi_a$, and let this function correspond to a function $\psi_a^{(+)}$.

We now calculate the mean of the operator $\dot{A} = \frac{1}{i\hbar}[A, H]$ in the state $\psi_a^{(+)}$:

$$(\psi_a^{(+)}, \dot{A}\psi_a^{(+)}) = \left(\psi_a^{(+)}, \frac{1}{i\hbar}[A, H_1]\psi_a^{(+)}\right). \tag{12.11}$$

Note that in general, this expression, unlike the analogous expression for the case of a discrete spectrum, does not vanish, since formally it is equal to a difference of two expressions each of which is infinite and thus meaningless.

Using the completeness property of the functions Φ_b, we write (12.11) in the form

$$\left(\psi_a^{(+)}\frac{1}{i\hbar}[A, H_1]\psi_a^{(+)}\right) = \frac{2}{\hbar}\sum_b A_b \operatorname{Im}(\psi_a^{(+)}\Phi_b)T_{ba} =$$

$$= \frac{2}{\hbar}\sum_b A_b \operatorname{Im} T_{ba}\left\{\delta_{ba} + \frac{T_{ba}^*}{E_a - E_b - i\varepsilon}\right\}, \tag{12.12}$$

where

$$T_{ba} \equiv (\Phi_b, H_1\psi_a^{(+)}) = (\psi_b^{(-)}, H_1\Phi_a)$$

determines the probability W_{ba} of a transition from state a to state b in unit time:

$$W_{ba} = \frac{2\pi}{\hbar}|T_{ba}|^2\delta(E_b - E_a). \tag{12.13}$$

Using the equality

$$\frac{1}{x - i\varepsilon} = P\frac{1}{x} + i\pi\delta(x),$$

we transform the right-hand side of identity (12.12) to the form

$$\frac{2}{\hbar}A_a \operatorname{Im} T_{aa} + \frac{2\pi}{\hbar}\sum_b A_b|T_{ba}|^2\delta(E_b - E_a). \tag{12.14}$$

If A is the unity operator, we obtain the ordinary "optical theorem" (although written in a different notation):

$$\frac{2}{\hbar}\operatorname{Im} T_{aa} + \frac{2\pi}{\hbar}\sum_b |T_{ba}|^2\delta(E_b - E_a) = 0. \tag{12.15}$$

Solving for $\operatorname{Im} T_{aa}$ and inserting in (12.14), we get

$$\left(\psi_a^{(+)}, \frac{1}{i\hbar}[A, H_1]\psi_a^{(+)}\right) = \frac{2\pi}{\hbar}\sum_b (A_b - A_a)|T_{ba}|^2(E_b - E_a) = \sum_b (A_b - A_a)W_{ba}. \tag{12.16}$$

This is the desired generalization of the "optical theorem". Expression (12.16) gives the probability of a change in A in unit time during scattering

(the right-hand side of the equality) as a function of the mean of a certain operator (the left-hand side of the equality).

Consider another particular case. Let $H_1 = V$, and for A we choose the momentum operator $\hat{\boldsymbol{p}}$. Relation (12.16) now takes the form

$$(\psi_a^{(+)}, (-\nabla V)\psi_a^{(+)}) = \sum_b (\boldsymbol{p}_b - \boldsymbol{p}_a) W_{ba}. \tag{12.17}$$

We have thus obtained the theorem on the momentum transfer in scattering, first proved in /82/.

Chapter 3

ANALYTICAL PROPERTIES OF THE WAVE FUNCTION

§ 13. ANALYTICAL PROPERTIES OF THE *S*-MATRIX

In the preceding chapter we showed that the scattering of particles in a potential field is completely described by the phase factors $S_l(k) = \exp(2i\delta_l(k))$.

If we know the exact form of the particle interaction potential, analytical or numerical solution of the Schroedinger equation will provide complete information on the system. Had this always been the case, we could leave with free conscience all the problems of quantum mechanics to electronic computers, and proceed with matters of more importance. However, the actual physical reality is far from this ideal state of things. In most cases, the particle interaction potential is simply not known. Moreover, the actual interaction between particles is apparently not described by potential forces.

Non-potential interactions are the subject of what is called quantum field theory. (Simple problems of this kind are considered in Chapter 8.) This theory, however, unlike quantum mechanics, is not free from internal difficulties. For example, calculation of certain quantities involves divergences (infinite, unbounded results). These divergences are apparently associated with improper description of interaction at very small distances.

Heisenberg /83/ attributed these difficulties to the use of nonobservables, such as $\psi(r)$, in the theory; a proper theory should deal only with observables, which include the functions $S_l(k) = \exp(2i\,\delta_l(k))$ forming the so-called S matrix (scattering matrix) /84/. The theory of the S-matrix is rapidly developing in recent years, especially in connection with the description of strong interactions of elementary particles. Particular attention is devoted to the construction of S-matrix theory using unitarity and analyticity properties. (Note that the importance of the analytical properties of the S-matrix was first emphasized by Kramers /85/ and Heisenberg /86/.) Numerous important advances were accomplished in this direction and various relations between experimental observables were established. Thus, the considerable progress in the theory of elementary particles is definitely attributed to ingenious application of the analytical properties of the S-matrix. Moreover, in case of quasistationary states and in some other cases, the behavior of a system can be described without introducing a particular interaction: it suffices to apply only general considerations on the position of the poles of the scattering amplitude.

The S-matrix formalism is generally regarded as precluding space-time description of processes. We should stress at this point that recent results /87, 88/ give actual prescriptions for space-time separation of

events within the framework of the S-matrix formalism. The applicability of intensity correlations to the determination of the scattering amplitude phase was demonstrated in /89—91/.

We will discuss the analytical properties of functions proceeding from the following general considerations:

(a) all the energy eigenvalues are real (a Hermitian Hamiltonian); the wave vector k is thus automatically real for continuum wave functions;

(b) elastic scattering is the only allowed process;

(c) the Hamiltonian is invariant under space inversion (when the space parity is conserved) and time reversal (when time parity is conserved).

Assumption (b) is needed so as to ensure that for given energy the radial Sch. Eq. has only one solution with given l. Conservation of time parity is equivalent to the requirement of a real Hamiltonian ($H^* = H$); hence it follows directly that if ψ is a solution of the Sch. Eq., ψ^* is also a solution.

We should note at this point that the space parity definitely changes in so-called weak interactions, as was conclusively demonstrated in 1957 /92, 93/; recent results also point to nonconservation of time parity /94/. Strong interactions, however, are believed to this day to conserve space and time parity. The following theorems are therefore fully applicable to strong interactions.

We will now consider the general properties of the functions $S_l(k)$ entering the scattering amplitude. *

We have seen that for potentials $U(r)$ which fall off at infinity faster than $1/r$, the Sch. Eq. has two solutions $\chi_{kl}^{(\pm)}$ which behave asymptotically as

$$\chi_{kl}^{(\pm)} \sim e^{\pm i\left(kr - \frac{\pi l}{2}\right)}$$

(the Coulomb potential case is not considered at this stage).

These functions can be formed into a solution which is regular at the origin:**

$$\chi_{kl} = a_l(k)\,\chi_{kl}^{(-)}(r) - b_l(k)\,\chi_{kl}^{(+)}(r), \tag{13.1}$$

where a_l and b_l are some constants dependent only on k. The function clearly vanishes for $r = 0$ if a_l and b_l satisfy the relation

$$\frac{b_l(k)}{a_l(k)} = \lim_{r\to 0} \frac{\chi_{kl}^{(-)}(r)}{\chi_{kl}^{(+)}(r)}. \tag{13.2}$$

From the definition of $S_l(k)$ we have

$$S_l(k) = \frac{b_l(k)}{a_l(k)}. \tag{13.3}$$

Let us consider the general invariance properties of the Sch. Eq. First, since it includes only the square of the wave vector k, the equation is

* A more detailed study of the analytical properties of wave functions and $S_l(k)$ will be found in /95—97/.

** This solution can be normalized using a k-independent condition, say $\lim_{r\to 0} r^{-(l+1)}\chi_l(r) = 1$. In this case, according to Poincaré's theorem /98/, $\chi_l(r)$ is an entire function of k^2.

invariant under a change in the sign of k. Thus if k is replaced by $-k$ in solution (13.1), the new function will also be a solution of the original equation. As the solution is single-valued, however, the two solutions χ_{kl} and χ_{-kl} may differ only by a constant factor. Since the asymptotic expression for the function $\chi_{kl}^{(\pm)}$ gives the relation

$$\chi_{kl}^{(\pm)}(r) = (-1)^l \chi_{-kl}^{(\mp)}(r), \tag{13.4}$$

we find, changing the sign of k in (13.1),

$$\frac{a_l(k)}{b_l(k)} = \frac{b_l(-k)}{a_l(-k)}.$$

Expression (13.3) yields the relation

$$S_l(k) = S_l^{-1}(-k). \tag{13.5}$$

Still another important formula can be derived if we notice that as the Sch. Eq. is real, the complex conjugate of any solution, $\chi_{kl}^*(r)$, is also a solution of the Sch. Eq. for real k. As the solution is unique, we again conclude that χ_{kl} and χ_{kl}^* may differ only by a constant factor, so that for real k

$$\frac{a_l(k)}{b_l(k)} = \frac{b_l^*(k)}{a_l^*(k)},$$

i.e.,

$$S_l(k) = (S_l^{-1}(k))^*. \tag{13.6}$$

This expression signifies that the two functions $S_l(k)$ and $(S_l^{-1}(k))^*$ coincide over the entire real axis in the complex k plane. According to the fundamental theorem of analytical continuation it follows that

$$S_l(k) = (S_l^*(k^*))^{-1} \tag{13.7}$$

in the entire complex k plane. The previous expressions establish a one-to-one correspondence between the $S_l(k)$ values in the different quadrants of the k plane (Figure 8): if the value of $S_l(k_0)$ at the point k_0 is S_0, we have

$$S_l(k_0^*) = \frac{1}{S_0^*}, \quad S_l(-k_0^*) = S_0^*, \quad S_l(-k_0) = \frac{1}{S_0}. \tag{13.8}$$

It is thus sufficient to have the form of $S_l(k)$ in one of the quadrants so as to be able to reconstruct the function $S_l(k)$ for the entire complex plane. The above relations indicate that at points symmetric about the imaginary axis, $S_l(k)$ takes on complex conjugate values. On the imaginary axis, $S_l(k)$ is thus a real function, and the phase $\delta_l(k)$ is a pure imaginary number:

$$\delta_l(\pm i|k|) = -\delta_l^*(\pm i|k|). \tag{13.9}$$

For points symmetric about the real axis, we have (13.7). Hence follows the known result: on the real axis $|S_l(k)| = 1$, and the phase $\delta_l(k)$ is real.

Let us now consider the singularities of $S_l(k)$. The regular solution (13.1) can be considered over the entire complex k plane, provided that $\chi_{kl}^{(\pm)}$ are treated as the analytical continuations of the corresponding functions for complex k. In particular, the regular solution will have the same form (13.1) on the imaginary axis. Let the potential $U(r)$ be such that a bound state of the particle exists for some negative energy $-E_0$ (or imaginary $k_0 = i|k_0|$). This means that the energy E_0 corresponds to a solution which is regular at the origin and falls off to zero as $e^{ik_0 r} = e^{-|k_0| r}$ at infinity. Since χ_{kl} is the only solution which is regular at the origin, the existence of a bound state implies that the coefficient $a_l(k)$ vanishes for $k = k_0 = i\sqrt{\frac{2m|E_0|}{\hbar^2}}$; the $\chi_{kl}^{(+)}$ at this point is regular at the origin. Similarly, as for all the k on the imaginary axis in the lower half plane ($k = -i|k|$)

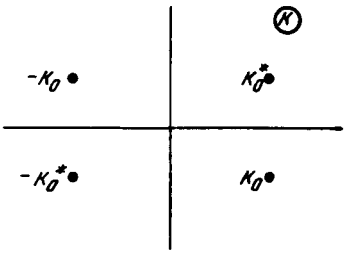

FIGURE 8.

$$\chi_{kl}^{(+)}(r) \to \infty \text{ for } r \to \infty, \quad \chi_{kl}^{(-)}(r) \to 0 \text{ for } r \to \infty,$$

the existence of a bound state implies the vanishing of the coefficient $b_l(k)$ at the point $k = -k_0$. This is a reflection of the previously mentioned general invariance property of the Sch. Eq. under sign reversal of k. Returning to (13.3) we come to the conclusion that a bound state corresponds to a pole of the function $S_l(k)$ situated on the imaginary axis in the upper halfplane at the point $k = k_0$.

In accordance with the previously discussed symmetry properties of $S_l(k)$, this pole corresponds to a zero of the function $S_l(k)$ at the point $k = -k_0$ on the imaginary axis in the lower halfplane. Notice also that although a bound state corresponds to a pole, the converse is not always true: not to every pole of $S_l(k)$ on the imaginary axis in the upper halfplane corresponds a bound state. There are so-called "false" or "redundant" poles of $S_l(k)$. We will yet return to this problem at a later stage.

It is readily seen that in the upper halfplane $S_l(k)$ may have poles only on the imaginary axis, so that in the lower halfplane the zeros also lie on the imaginary axis only. Indeed, apart from a common factor, the regular solution (13.1) can be written either as

$$\chi_{kl}(r) = \chi_{kl}^{(-)}(r) - S_l(k)\,\chi_{kl}^{(+)}(r), \tag{13.10}$$

or as

$$\chi_{kl}(r) = S_l^{-1}(k)\,\chi_{kl}^{(-)} - \chi_{kl}^{(+)}. \tag{13.10'}$$

If $S_l(k)$ had a pole at a point $k = k_0$ in the upper halfplane not on the imaginary axis, the solution (13.10') would contain only the function χ_{kl}^{+}, which falls off exponentially at infinity:

$$\chi_{kl}(r) \sim -(-i)^l e^{ik_0 r} = -(-i)^l e^{-(-ir\,\mathrm{Re}\,k_0 + r\,\mathrm{Im}\,k_0)}.$$

But the function $\chi_{kl}(r)$ is by definition regular at the origin, and therefore at the point k_0 this solution would satisfy the two boundary conditions (1.7), i.e., the complex quantity $\frac{\hbar^2 k_1^2}{2m}$ would be an eigenvalue of the Sch. Eq. This is impossible, since any physical potential is real and all the energy eigenvalues are real.

The requirement of a real potential is thus responsible for the concentration of the poles of $S_l(k)$ on the imaginary axis in the upper halfplane. In the lower halfplane, however, no restriction is imposed on the position of the poles, and they may be distributed at random. These conclusions remain in force even if the interaction forces are not potential. The main thing is that the Hamiltonian should be Hermitian.

This theorem can be given an alternative, more formal proof. Consider the time-dependent Sch. Eq. and its conjugate:

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi + U\psi,$$
$$-i\hbar \frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi^* + U\psi^*.$$

The first equation is multiplied by ψ^*, the second by ψ, and one is subtracted from the other. We get

$$i\hbar \frac{\partial}{\partial t}|\psi|^2 = -\frac{\hbar^2}{2m}\nabla(\psi^*\nabla\psi - \psi\nabla\psi^*).$$

Integration of this equation over an arbitrary volume V enclosed within a surface S gives the law of particle number conservation:

$$\frac{\partial}{\partial t}\int_V |\psi|^2 dr = \oint_S dS \frac{i\hbar}{2m}(\psi^*\nabla\psi - \psi\nabla\psi^*). \qquad (13.11)$$

Let now $S(k)$ have a pole at some point $k_0 = k_1 + ik_2$. The wave function at this point has the form

$$\psi = \frac{1}{r}\chi(r)e^{-\frac{iEt}{\hbar}} \sim \frac{1}{r}e^{i(k_1+ik_2)r - \frac{i\hbar}{2m}(k_1^2 - k_2^2 + 2ik_1k_2)t}.$$

Inserting this expression in (13.11), we choose the volume V as the inside of a sphere of radius $r = R$, where R is sufficiently large so that on the surface of the sphere we may use the asymptotic expression for the wave function. Elementary manipulations give

$$k_1 k_2 \int_0^R |\chi(r)|^2 dr = -\frac{k_1}{2R^2}e^{-2Rk_2}.$$

Since there is a minus sign in the right-hand side, this equality is satisfied only if

(a) $k_1 = 0$, i.e., the pole of $S(k)$ lies on the imaginary axis,

(b) $k_1 \neq 0$, $k_2 < 0$, i.e., the pole of $S(k)$ lies in the lower halfplane.

This completes the proof of the theorem.

The only constraint on the position of the poles in the lower halfplane is that they should occur in pairs symmetrically about the imaginary

axis.* The zeros of $S_l(k)$ in the lower halfplane, however, may lie only along the imaginary axis. This follows from (13.5).

Poles in the upper halfplane correspond as a rule to bound states of particles in the field $U(r)$. For poles in the lower halfplane the regular (at the origin) wave function has the asymptotic form

$$\left.\begin{aligned} \chi_{kl}(r) \sim -(-i)^l e^{ikr} = -(-i)^l e^{ir\,\mathrm{Re}\,k + r\,|\,\mathrm{Im}\,k\,|}, \\ \chi_{kl}(r) \to \infty \text{ for } r \to \infty, \end{aligned}\right\} \tag{13.12}$$

i.e., it diverges at infinity.

This wave function thus does not satisfy the boundary condition at infinity and would seem to be physically meaningless. This is not quite so, however. In Chapter 5 we will see that to every pole of $S_l(k)$ in the lower halfplane corresponds a so-called quasistationary state of the particle in the field $U(r)$, i.e., a state which, once formed, will have a finite lifetime τ.

Let us sum up what we have learned on the topography of the function $S_l(k)$ in the complex plane. This function is analytical in the entire complex k plane, with the possible exception of isolated singularities and cuts. In the upper halfplane it may have poles on the imaginary axis only. Some of these poles correspond to bound states, other are "false" poles. In the next section we will give a prescription for identifying the "false" poles. $S_l(k)$ may have zeros in the upper halfplane and corresponding poles in the lower halfplane. On the imaginary axis $S_l(k)$ is real and on the real axis its modulus is equal to unity. If the wave vector k is replaced by energy, we should remember that the k plane is mapped onto a two-sheet E plane. Bound states correspond to poles on the left semiaxis in the upper E plane. The poles on the lower sheet of the E plane correspond to quasistationary states.

In what follows we will require the symmetry properties of scattering phases. On the real axis the phase δ is real. By (13.5) we see that for real k

$$\delta_l(k) = -\delta_l(-k). \tag{13.13}$$

Wave functions normalized to $\delta(k-k')$ have the asymptotic expression

$$\chi_{kl} \sim \sqrt{\frac{2}{\pi}} \sin\left(kr + \delta(k) - \frac{\pi l}{2}\right).$$

Using this expression, we can readily verify that as the sign of k changes, the wave functions behave in the following way:

$$\chi_{k,l}(r) = (-1)^{l+1}\chi_{-k,l}(r). \tag{13.14}$$

We have mentioned in the preceding that $S_l(k)$ is an analytic function in the complex k plane. This holds true for any potential and is a consequence

* For potentials vanishing for $r > R$ there is an infinity of such poles /99–101/; in this case the distribution of the distant poles is completely determined by the behavior of the potential for $r \to R$. The poles in case of a rectangular box were treated in detail in /102/.

of the principle of physical causality. * In other words, the cause must precede the effect. This is an inevitable prerequisite of any physical theory, and it is found to have very far-reaching consequences. We will now try to sketch a rough outline of the formal results emerging from the causality principle.

We write the expression for the wave function for given energy E at some distance $r = a$ outside the effective range of the potential:

$$(e^{-ika} - S(E)\, e^{ika})\, e^{-\frac{iEt}{\hbar}}.$$

The first term corresponds to the incoming wave and the second to the outgoing wave. A spatially localized wave packet is given by

$$\int_0^\infty dE' \,(f(E')\, e^{-ik'a} - g(E')\, e^{ik'a})\, e^{-\frac{iE't}{\hbar}},\ g(E') = S(E')\, f(E'). \tag{13.15}$$

The wave packet describing the incoming waves is clearly

$$\Phi_{\text{in}}\ (a, t) = \int_0^\infty dE' f(E')\, e^{-ik'a - \frac{iE't}{\hbar}},$$

and the wave packet of the outgoing waves is

$$\Phi_{\text{out}}\ (a, t) = \int_0^\infty dE' g(E')\, e^{ik'a - \frac{iE't}{\hbar}}.$$

Since the system is linear and the amplitude of the divergent outgoing waves is fully determined by the incident wave, we have the following relation between the two amplitudes:

$$\Phi_{\text{out}}\ (a, t) = \int_{-\infty}^{\infty} H(t - t')\, \Phi_{\text{in}}\ (a, t')\, dt', \tag{13.16}$$

where H is some transformation kernel.

It is here that the causality principle enters the discussion: the amplitude of the outgoing wave at the time t can depend on $\Phi_{\text{in}}(t')$ only if $t > t'$. We must therefore have

$$H(t - t') = 0 \quad \text{for} \quad t' > t. \tag{13.17}$$

Introducing the Fourier component $h(\omega)$ of the operator H,

$$H(\tau) = \int_{-\infty}^{\infty} d\omega e^{-i\omega\tau} h(\omega), \tag{13.18}$$

we easily find from (13.15) – (13.18) that

$$h(E) = \frac{1}{2\pi} e^{2ika} S(E). \tag{13.19}$$

* This idea was first advanced in /103/, but the original proof is not fully rigorous. The rigorous proof first given by Van Kampen /104/ requires knowledge of comparatively fine theorems of the theory of analytic functions.

Inverting (13.18), we get

$$e^{2ika}S(E) = +\int_{-\infty}^{\infty} e^{iE\tau}H(\tau)\,d\tau.$$

In the general case, this expression sheds no light on the properties of $S(E)$. By the causality principle, however (see (13.17)), we know that $H(\tau) = 0$ for $\tau < 0$. The integration should therefore start from zero:

$$e^{2ika}S(E) = +\int_{0}^{\infty} e^{iE\tau}H(\tau)\,d\tau. \qquad (13.20)$$

In this case the function in the right-hand side is clearly analytical in the upper E halfplane, where $e^{iE\tau}$ decays exponentially. In the k plane this corresponds to the first quadrant. Thus, using the symmetry properties of $S(k)$, we find that $S(k)$ is analytic in all the quadrants. The exponential factor e^{2ika} in (13.20) accounts for the phase lead of the wave reflected from the spherical surface $r = a$ relative to the wave passing through the scattering center /105/ (the corresponding path length difference is $2a$).

For a plane wave scattered at a finite angle θ we should choose the shortest path (corresponding to maximum phase lead) through the scattering sphere which reaches the observer at an angle θ (Figure 9). This path length is less by $2a\sin\frac{\theta}{2}$ than the length of the path through the scattering center. Therefore, in the upper E halfplane, it is the function $e^{2ika\sin\frac{\theta}{2}}f(E,\theta)$ that is analytic, and not the scattering amplitude $f(E, \theta)$. Hence it is clear that the simplest analytical properties are characteristic of $f(E, 0)$ (it is analytic in the upper E halfplane).

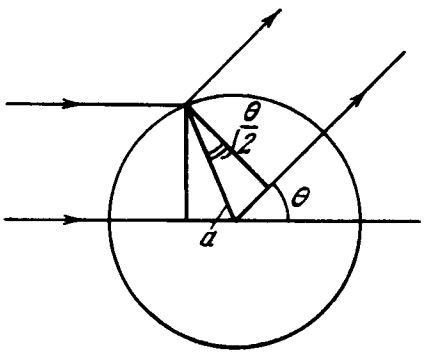

FIGURE 9.

The causality principle can be applied to derive the analyticity properties of the scattering amplitude from momentum transfer /106/. Note that the validity of our assertions on analyticity is independent of the particular form of the potential for $r < a$. Moreover, even the assumption that the wave function inside the interaction range ($r < a$) satisfies the Sch. Eq. is unnecessary. In other words, the analyticity of $S(E)$ in the upper E halfplane is a direct consequence of the causality principle alone. This problem is discussed in /107, 108/.

§ 14. "FALSE" POLES

We have already mentioned that in the upper halfplane $S_l(k)$ may have so-called "false" poles* on the imaginary axis, which do not correspond to

* The existence of these poles was first pointed out by Ma /109/ [who called them "redundant"].

physical bound states. The nature of the "false" poles can be understood if we recall the definition of $S_l(k)$: we started with two independent solutions of the Sch. Eq. $\chi_{kl}^{(+)}$ and $\chi_{kl}^{(-)}$ with asymptotic behavior $\chi_{kl}^{(\pm)} \sim e^{\pm i\left(kr - \frac{\pi l}{2}\right)}$ for large r; since we are dealing with scattering problems, the asymptotics is computed for positive k. Then these two functions are formed into a solution which is regular at the origin,

$$\chi_{kl}(r) = \chi_{kl}^{(-)} - S_l(k)\,\chi_{kl}^{(+)}.$$

For this function to vanish at $r = 0$ it is necessary and sufficient that $S_l(k)$ have the form (13.2). The points in the upper k halfplane where the denominator of (13.2) ($\chi_{kl}^{(+)}(0)$) vanishes correspond to bound states. These points lie on the imaginary axis in the upper halfplane. In addition to poles of this kind, $S_l(k)$ may have poles associated with the poles of the function $\chi_{kl}^{(-)}(r)$. By this we mean those points of the complex k plane where $\chi_{kl}^{(-)}$ as a function of k is identically infinite for all r. These points, clearly do not correspond to any bound states.

Consider the particular case of a potential $V(r) = -V_0 e^{-\frac{r}{a}}$. The Sch. Eq. takes the form

$$\chi_k''(r) + [k^2 + V_0 e^{-\frac{r}{a}}]\,\chi_k(r) = 0 \tag{14.1}$$

and substitution of a new variable $y = 2a\sqrt{V_0}\,e^{-\frac{r}{2a}}$ reduces it to Bessel's equation

$$\chi_k''(y) + \frac{1}{y}\chi_k'(y) + \left[1 - \frac{(ip)^2}{y^2}\right]\chi_k(y) = 0, \tag{14.2}$$

where $p = 2ka$. As two independent solutions of this equation we may take Bessel's functions $J_{ip}(y)$ and $J_{-ip}(y)$, defined in the usual way:

$$J_\nu(y) = \sum_{m=0}^{\infty} (-1)^m \left(\frac{y}{2}\right)^{\nu+2m} \frac{1}{m!\,\Gamma(m+\nu+1)}. \tag{14.3}$$

Using this expansion, we easily find the asymptotic form of the functions $J_{\pm ip}(y)$ for $r \to \infty$ (i.e., when $y \to 0$)

$$J_{\pm ip}(y) \underset{y\to 0}{\sim} (\sqrt{a^2V_0})^{\pm ip} \frac{e^{\mp ikr}}{\Gamma(1 \pm ip)}. \tag{14.4}$$

We can thus define the functions $\chi_k^{(\pm)}(r)$:

$$\left.\begin{aligned} &\chi_k^{(\pm)}(r) = \Gamma(1 \mp ip)\,(\sqrt{a^2V_0})^{\pm ip}\, J_{\mp ip}(2a\sqrt{V_0}e^{-\frac{r}{2a}}) \\ &\chi_k^{(\pm)}(r) \sim e^{\pm ikr} \text{ for } r \to \infty. \end{aligned}\right\} \tag{14.5}$$

Using definition (13.2), we find

$$S(k) = \frac{\Gamma(1+ip)}{\Gamma(1-ip)}(\sqrt{a^2V_0})^{-2ip}\frac{J_{ip}(y_0)}{J_{-ip}(y_0)}, \quad y_0 = 2a\sqrt{V_0}. \tag{14.6}$$

The case of attraction corresponds to positive values of V_0, i.e., the argument y_0 of Bessel's functions is a positive number. For real k, by

definition, $\delta(k)$ is also real and we clearly have $|S(k)| = 1$. On the positive imaginary axis $ip = -i2ak = +2a|k|$ and $S(k)$ has poles at the points k_n, where

$$J_{2|k_n|a}(2a\sqrt{V_0}) = 0. \tag{14.7}$$

These poles clearly correspond to bound states, since the wave function

$$\chi_k(r) = \frac{1}{S(k)}\chi_k^{(-)} - \chi_k^{(+)} \xrightarrow[k \to k_n]{} -\chi_{k_n}^{(+)}(r);$$
$$\chi_{k_n}^{(+)}(r) \sim e^{-|k_n|r},\ r \to \infty;\ \chi_{k_n}^{(+)}(r) \to 0,\ r \to 0$$

satisfies the two boundary conditions at these points.

In addition to poles of this kind, $S(k)$ also has poles at the points

$$1 + ip = 1 - 2a|k_m| = -m \quad (m = 0, 1, 2, 3, 4, \ldots),$$

where $\Gamma(1 + ip)$ goes to infinity. This infinite sequence of poles does not correspond to any bound states, and they are thus "false" and "redundant". To verify this, we write the expression for the wave function. Using (14.5), we find

$$\chi_k(r) = (\sqrt{a^2V_0})^{-ip}\Gamma(1 + ip)\left[J_{ip}(y) - \frac{J_{ip}(y_0)J_{-ip}(y)}{J_{-ip}(y_0)}\right]. \tag{14.8}$$

At the points $k = k_m$ the factor $\Gamma(1 + ip)$ goes to infinity. The expression in brackets in (14.8), however, vanishes on account of the well known property of Bessel's functions $J_{-l}(y) = (-1)^l J_l(y)$, where l is an integer.

Using the expression for Bessel's function with negative index,

$$J_{-\nu}(y) = \cos \pi\nu J_\nu(y) - \sin \pi\nu N_\nu(y),$$

where $N_\nu(y)$ is Neumann's function, we obtain without difficulty

$$\chi_{k_m}(r) = \lim_{k \to k_m} \chi_k(r) = -\frac{\pi}{m!}(a\sqrt{V_0})^{m+1}\left[N_{m+1}(y) - J_{m+1}(y)\frac{N_{m+1}(y_0)}{J_{m+1}(y_0)}\right]. \tag{14.9}$$

This solution is regular at the origin, but for $r \to \infty$ it increases exponentially, $\chi_{k_m}(r) \sim e^{k_m r}$ for $r \to \infty$, and therefore does not correspond to any bound state.

Let us now try to elucidate the general reasons for the formation of "false" poles. We already know that they are associated with the pole of the function $\chi_k^{(-)}$. The function $\chi_k^{(-)}$ is defined as that solution of the Sch. Eq. which for large r behaves on the real k axis as e^{-ikr}. If, however, $\chi_k^{(-)}$ is infinite somewhere in the complex k plane, the asymptotic expression $\chi^{(-)} \sim e^{-ikr}$ breaks down when we move from the real axis into the complex plane, since e^{-ikr} is bounded for all k, except $k = i\infty$. The asymptotic form of this function is not conserved if the exact expression for this function, besides the term e^{-ikr}, also contains other terms which, though safely ignorable on the real axis, are not so in the entire complex plane.

In the case under discussion (an exponential potential), these terms have the form

$$\chi_k^{(-)} = e^{-ikr}\left(1 + \sum_{m=1}^{\infty}(-1)^m (a^2V_0)^m \frac{\Gamma(1 + ip)}{m!\,\Gamma(m + ip + 1)} e^{-\frac{mr}{a}}\right). \tag{14.10}$$

On the real axis, for sufficiently large r, the second term in (14.10) is always ignorable. On passing to the complex plane, the situation is essentially altered by the poles of the gamma function on the negative semiaxis. At the poles the second term in (14.10) is dominant compared to unity, despite the smallness of the exponential terms $e^{-\frac{mr}{a}}$.

We can now answer the question, when do the "false" poles form? Indeed, we see from the preceding, that a sufficient condition for the absence of "false" poles is the applicability of the asymptotic expression $\chi_k^{(-)} \sim e^{-ikr}$ in the entire halfplane, since in this case $\chi_k^{(-)}$ has no poles. Hence it follows directly that if the potential $V(r)$ is identically zero outside a sphere of any arbitrarily large radius R, there are no "false" poles.* The point is that in this case for $r > R$ the function $\chi_k^{(-)}$ (like $\chi_k^{(+)}$) is a superposition of Bessel's functions for which the validity of the asymptotic expressions in the entire complex plane is proved without difficulty (e.g., using expression (14.3) which is valid everywhere). Thus, $\chi_k^{(-)}$ has no poles anywhere in this case, and no "false" poles form. This is readily checked for our example of an exponential potential by cutting it off for some $r = R$. All the poles corresponding to bound states are virtually unaffected, whereas the "false" poles disappear.

We thus come to the following remarkable conclusion: when a potential is cut off, all physically meaningless "false" poles disappear, whereas the "physical" poles corresponding to bound states are virtually unaffected. The latter point is quite understandable. If we cut off the potential somewhere far away, where it is small, this can hardly alter the physical properties of the system, in particular the energy and the wave functions of the bound states. A situation of this kind, when some sort of a cutoff essentially simplifies the analytical properties of functions without affecting their physical meaning, is often encountered in modern theoretical physics. The example of "false" poles is probably the simplest in this respect as far as mathematics is concerned.

The above considerations suggest the following prescription for the calculation of the energy of bound states in case of potentials which do not vanish identically at infinity: the potential should be cut off at some $r = R$, the position of the poles of $S_l(k)$ in the upper k halfplane should be found, and R should then be allowed to go to infinity; the limits $k_n(R)|_{R\to\infty}$ give the energy of the bound states.

The problem of the "false" poles of the S-matrix is closely related to the problem of reconstruction of the potential $U(r)$ from the scattering phase $\delta_l(k)$, e.g., the s-phase $\delta_0(k)$. In distinction from the case of classical mechanics, where scattering data completely determine the potential $U(r)$ /110/, the solution of this problem in quantum mechanics is not single-valued. Bargmann /111/ gave examples of various potentials and even families of potentials which all produce the same expression for the scattering phase $\delta_0(k)$. Different potentials $U(r)$ in general correspond to different subdivisions of all the poles of $S_0(k) = e^{2i\delta_0(k)}$ into "true" and "false". This property, and some other properties of Bargmann potentials, are treated in /112/ (see also /113/). It is remarkable that for some potentials /114/ the phase $\delta_0(k) \equiv 0$, i.e., no s-state scattering is observed for all k.

* It can also be shown /101/ that "false" poles are absent for potentials which fall off at infinity faster than any exponential $e^{-\mu r}$.

The determination of potential from scattering phases was completely solved by Gel'fand and Levitan /115/ and by Marchenko /116, 117/, who showed that for single-valued recovery of the potential, the scattering phases should be supplemented by the energies of the bound states and the coefficients A_n which specify the asymptotic behavior of the corresponding wave functions for large r:

$$\psi_n \underset{r\to\infty}{\sim} A_n \frac{e^{-\varkappa_n r}}{r}.$$

§ 15. PROPERTIES OF RESIDUES OF $S_l(k)$

Consider a bound state of momentum l and binding energy $E_0 = \frac{\hbar^2\varkappa^2}{2m}$. The wave function of this state is assumed to be normalized:

$$\int_0^\infty |\chi_l(r)|^2 dr = 1.$$

We first consider the case when for $r \to \infty$ the potential $U(r)$ falls off faster than $1/r$. Then χ_l behaves for large r as

$$\chi_l \sim A_l e^{-\varkappa r}, \tag{15.1}$$

where A_l is a constant determined by the form of the potential.

As we know, $S_l(k)$ has a pole at the point $k = i\varkappa$:

$$S_l(k) = \frac{C_l}{k - i\varkappa}. \tag{15.2}$$

A universal relationship can be established between C_l — the residue of S_l at the pole — and the constant A_l entering the asymptotic expression for the normalized wave function of the bound state, *

$$C_l = (-1)^{l+1} i |A_l|^2. \tag{15.3}$$

Making use of this relation, one can reach certain conclusions concerning the properties of the bound state from the behavior of scattering phases. In field theories analogous relations are used to determine the coupling constants.

We can now proceed with the proof of (15.3). The solution which is regular at the origin and behaves asymptotically as

$$\chi_{kl}(r) \sim \text{const} \cdot \left[e^{-i\left(kr - \frac{\pi l}{2}\right)} - S_l e^{i\left(kr - \frac{\pi l}{2}\right)}\right]$$

* This relation was first derived by Heisenberg /83/ and Möller /118/; also see /119/.

should coincide, apart from a constant factor, with the function χ_l of the bound state for $k = i\varkappa$. We normalize χ_{kl} so that this factor is unity:

$$\lim_{k \to i\varkappa} \chi_{kl} = \chi_l.$$

This condition clearly corresponds to the normalization

$$\chi_{kl} = A_l \left(e^{ikr} - \frac{(-1)^l}{S_l} e^{-ikr} \right). \tag{15.4}$$

Consider an infinitesimal neighborhood of the pole:

$$\begin{gathered} k = i\varkappa + \varepsilon, \quad \varepsilon \to 0, \quad \varepsilon > 0, \\ \chi_{kl}(r) = A_l \left(e^{ikr} - \frac{(-1)^l}{C_l} \varepsilon e^{-ikr} \right). \end{gathered} \tag{15.4'}$$

We will use the law of particle number conservation which is readily seen to apply to both real and complex k:

$$\frac{\partial}{\partial t} \int_0^R \left| \chi_{kl} e^{-\frac{iEt}{\hbar}} \right|^2 dr = \frac{i\hbar}{2m} \left| e^{-\frac{iEt}{\hbar}} \right|^2 (\chi_{kl}^* \chi_{kl}' - \chi_{kl} \chi_{kl}^{*\prime}) \Big|_{r=R}. \tag{15.5}$$

First consider the left-hand side of (15.5). The energy E is a complex number in our case:

$$E = \frac{\hbar^2}{2m} (i\varkappa + \varepsilon)^2 = -\frac{\hbar^2}{2m} (\varkappa^2 - \varepsilon^2) + i \frac{\hbar^2}{m} \varkappa\varepsilon,$$

so that

$$\frac{\partial}{\partial t} \int_0^R |\chi_{kl}|^2 e^{\frac{2\hbar\varkappa\varepsilon t}{m}} dr \xrightarrow[\varepsilon \to 0]{} \frac{2\hbar}{m} \varkappa\varepsilon \left(1 - |A_l|^2 \frac{1}{2\varkappa} e^{-2\varkappa R} \right). \tag{15.6}$$

Here the radius R is taken sufficiently large to justify using the asymptotic expression (15.1) for the wave function.

Now consider the right-hand side of (15.5). The residue C_l is clearly a pure imaginary quantity:

$$C_l^* = -C_l.$$

This follows from the fact that δ_l is real for all imaginary k (see § 13). Using this fact and inserting (15.4') in the right-hand side of (15.5), we obtain to terms linear in ε

$$\frac{i\hbar}{2m} \left| e^{-\frac{iEt}{\hbar}} \right|^2 (\chi_{kl}^* \chi_{kl}' - \chi_{kl} \chi_{kl}^{*\prime}) \Big|_{r=R} \to \varepsilon \frac{2\hbar\varkappa}{m} \left\{ -\frac{i(-1)^l}{C_l} |A_l|^2 - \frac{|A_l|^2}{2\varkappa} e^{-2\varkappa R} \right\}.$$

Comparison with (15.6) yields

$$C_l = (-1)^{l+1} i |A_l|^2,$$

which completes the proof.

Relation (15.3) can be generalized to the case of a potential with a Coulomb tail, $U(r) \sim -\frac{\alpha}{r}$ for $r \to \infty$ /120/. The asymptotic expression for the wave function in this case is

$$\chi_l(r) \sim A_l (\varkappa r)^{\eta} e^{-\varkappa r}, \quad \eta = \frac{m\alpha}{\hbar^2 \varkappa}, \tag{15.1'}$$

and relation (15.3) takes the form

$$C_{\varkappa l} = (-1)^{l+1} i 2^{-2\eta} e^{-i\pi\eta} |A_{\varkappa l}|^2. \tag{15.3'}$$

This theorem makes it possible to establish the upper bound for the absolute value of the residues C_l. Indeed, suppose that we know that the potential $U(r)$ has a finite range R; in this case for $r > R$ the wave function of the bound state must have the form of the free-motion wave function

$$\chi_l(r) = A_l k r h_l^{(1)}(kr) = A_l i^{l+\frac{3}{2}} \sqrt{\frac{\pi |k_{nl}| r}{2}} H^{(1)}_{l+\frac{1}{2}}(i|k_{nl}|r) \sim A_{nl} e^{-|k_{nl}|r}. \tag{15.7}$$

The normalizing constant A_l clearly depends on the form of the potential $U(r)$. We rewrite the normalization condition in the form

$$1 = \int_0^{\infty} |\chi_l(r)|^2 dr = \int_0^{R} |\chi_l|^2 dr + k^2 \int_R^{\infty} |A_l|^2 |h_l^{(1)}|^2 r^2 dr. \tag{15.7'}$$

All the terms in the right-hand side are positive. We therefore obtain the inequality

$$|A_{nl}|^2 \leqslant \frac{1}{k^2 \int_R^{\infty} |h_l^{(1)}|^2 r^2 dr} = \left\{ \frac{\pi k_{nl} (-1)^{l+1}}{4} R^2 \left[-\left(H^{(1)}_{l-\frac{1}{2}}(k_{nl}R) \right)^2 + H^{(2)}_{l-\frac{1}{2}} H^{(1)}_{l+\frac{3}{2}} \right] \right\}^{-1}. \tag{15.8}$$

For $l = 0$ and $l = 1$ we thus obtain*

$$|A_0|^2 \leqslant 2\varkappa e^{2\varkappa R}, \tag{15.9}$$

$$|A_1|^2 \leqslant 2\varkappa e^{2\varkappa R} \frac{1}{1+\frac{2}{\varkappa R}}. \tag{15.9'}$$

The upper bound for $|A_l|^2$ and correspondingly for C_l is thus determined by the range R of the potential, the energy of the bound state, and the particle mass m.

In the limit for $R \to 0$, (15.9) takes the form

$$|A_0|^2 \leqslant 2\varkappa \quad \text{and} \quad |A_1|^2 \leqslant 0. \tag{15.10}$$

$|A_1|^2$ is of course nonnegative. Therefore, the above inequality implies that a potential with a range $R \to 0$ precludes existence of bound states with $l \neq 0$. The inequality for A_0 in the case of a Sch. Eq. with singular potential reduces to equality, since the wave function of the bound state has the

* These inequalities were derived in /121/.

form $Ae^{-\varkappa r}$ in the entire space and the first term in (15.8) identically vanishes, so that

$$|A_0|^2 = 2|\varkappa|.$$

If the range R of the potential is finite, $|A_0|^2$ is strictly less than $2\varkappa e^{2\varkappa R}$. This fact can be used in estimating the range of the potential from scattering data. Indeed, given the scattering phase for real k, we can extrapolate the function $e^{2i\delta}$ for imaginary k. This will give the residue C_l, and thus $|A|^2$. If we find that $|A_0|^2 \leqslant 2|\varkappa|$, a point potential is possible; if, however, $|A_0|^2 > 2|\varkappa|$, the potential has a finite range.

Consider, for example, the interaction between a neutron and a proton in the triplet state. The scattering phase for a state with zero orbital momentum is given by /122/

$$k \cot \delta = -\frac{1}{a} + \frac{1}{2} r_0 k^2, \tag{15.11}$$

where a is the scattering length ($a = 5.4 \cdot 10^{-13}$ cm), and $r_0 = 2 \cdot 10^{-13}$ cm is the so-called effective radius. In the case under discussion, the neutron and the proton possess a bound state (a deuton) with binding energy $\varepsilon = 2.2$ MeV. Using (15.11), we obtain the following expansion near the pole at $k = k_0 = i|k_0|$, which corresponds to a bound state:

$$S = e^{2i\delta} \to -\frac{2i|k_0|}{(k-k_0)(1-2r_0/a)^{1/2}}. \tag{15.12}$$

Hence we find (see (15.3)) that the normalizing constant of the bound-state wave function is

$$|A|^2 = \frac{2|k_0|}{(1-2r_0/a)^{1/2}} \approx \frac{2|k_0|}{1-r_0|k_0|}, \tag{15.13}$$

and expression (15.9) gives the following inequality for the interaction range R:

$$e^{2|k_0|R} > \frac{1}{1-r_0|k_0|}. \tag{15.14}$$

Inserting numerical values for $|k_0|$ and r_0, we finally obtain $R > 1.35 \cdot 10^{-13}$cm.

The interaction range R can be estimated by an alternative technique. In what follows we will prove the following strict inequality:*

$$\frac{d\delta}{dk} + R - \frac{1}{2k}\sin(2kR + 2\delta) > 0. \tag{15.15}$$

Inserting the phase δ from (15.11) and taking the limit $k \to 0$, we see that (15.15) reduces to

$$R\left[1 - \frac{R}{a} + \frac{1}{3}\left(\frac{R}{a}\right)^2\right] > \frac{r_0}{2}. \tag{15.16}$$

* This inequality was first obtained by Wigner /123/ proceeding only from the causality principle.

We now proceed to prove (15.15). The Sch. Eq. for two close energy values E and E_1 are

$$\chi_E'' - \frac{2m}{\hbar^2}(U - E)\chi_E = 0,$$

$$\chi_{E_1}'' - \frac{2m}{\hbar^2}(U - E_1)\chi_{E_1} = 0.$$

Multiplying the first equation by χ_{E_1}, the second by χ_E, and subtracting one from the other, we obtain

$$(\chi_{E_1}\chi_E' - \chi_E\chi_{E_1}')' = \frac{2m}{\hbar^2}(E_1 - E)\chi_E\chi_{E_1}.$$

Integrating this equality over r from 0 to R and taking the limit as $E_1 \to E$, we find

$$\int_0^R \chi_E^2\, dr = \frac{\hbar^2}{2m}\lim_{E_1 \to E}\frac{1}{E_1 - E}(\chi_{E_1}\chi_E' - \chi_{E_1}'\chi_E)|_{r=R}. \tag{15.17}$$

Since for $r = R$ the potential is zero, the wave functions χ can be expressed in the form

$$\chi_E \approx \sqrt{\frac{2}{\pi}}\sin(kr + \delta).$$

Inserting this expression in (15.17) we obtain after elementary manipulations /124/

$$\int_0^R \chi_E^2\, dr = \frac{1}{\pi}\left\{\left(R + \frac{d\delta}{dk}\right) - \frac{1}{2k}\sin 2(kR + \delta)\right\}. \tag{15.18}$$

The left-hand side is a priori positive. The right-hand side is thus also positive, so that inequality (15.15) applies.

In conclusion of this section note that the above results apply only to the Sch. Eq. with a potential. They should be modified if we are dealing with a system of particles capable of mutual transformations. This problem is discussed in more detail in Chapter 8.

§ 16. DISPERSION RELATIONS

We will now consider a few examples when the general analyticity properties of $S_l(k)$ give useful relations for the wave function.

We have already mentioned that $S_l(k)$ are analytic functions of k whose poles in the upper halfplane are concentrated on the imaginary axis only. Some of these poles correspond to bound states, but there are also some redundant poles.

Near the n-th pole

$$S_l(k) = \frac{C_{nl}}{k - k_{nl}} \text{ and } \frac{S_l'(k)}{S_l(k)} = 2i\delta_l'(k) = -\frac{1}{k - k_{nl}}. \tag{16.1}$$

We also know that in the lower halfplane the poles occur in pairs, symmetrically about the imaginary axis; each pair corresponds to a so-called quasistationary state. Moreover, poles may also lie on the imaginary axis in the lower halfplane. These poles correspond to the so-called virtual states. Each of these poles corresponds to a zero of $S_l(k)$ in the upper halfplane. Near each of these zeros

$$S_l(k) = \alpha_{ml}(k - k_{ml}) \quad \text{and} \quad \frac{S_l'}{S_l} = 2i\delta_l'(k) = \frac{1}{k - k_{ml}}. \tag{16.2}$$

Let us first consider the case of an S-matrix with a finite number of poles. Consider N_b bound states, N_r redundant poles, N_q quasistastationary states, and N_v virtual states. In the upper halfplane there are thus $(N_b + N_r)$ points where (16.1) is satisfied and $(2N_q + N_v)$ points where (16.2) is satisfied.

Everywhere else $S_l(k)$ is bounded. Consider the integral

$$I = 2i\int_{-\infty}^{\infty} \delta_l'(k)\,dk = 4i\int_0^{\infty} \delta_l'(k)\,dk = 4i\,(\delta_l(\infty) - \delta_l(0)).$$

For $|k| \to \infty$, $S_l(k) \to 1 + \frac{2i\beta}{k}$; $\beta = \text{const}$ (see Chapter 4). This means that the phase $\delta_l(k) \to p\pi + \beta/k$, where p is an integer and $\delta'(k) \sim k^{-2}$. We can therefore complete the integration contour in the upper halfplane and calculate the integral, as all the poles and their residues in the upper halfplane are known:

$$I = 2\pi i\,(2N_q + N_v - N_b - N_r).$$

Equating the two expressions for I, we obtain a relation between the phase at infinity and the number of bound and quasistationary states (we take $\delta_l(0) = 0$)

$$\delta_l(\infty) - \delta_l(0) = \delta_l(\infty) = \frac{\pi}{2}(2N_q + N_v - N_b - N_r). \tag{16.3}$$

In the general case, e.g., for a potential which vanishes for $r > R$, there is an infinite number of poles. The number of bound states, on the other hand, is mostly finite. The above reasoning breaks down in this case, since the integral over the upper semicircle is no longer ignorable. Nevertheless, Levinson /126/ showed that in this case also one can derive an expression relating the phase at infinity to the number of bound states:

$$\delta_l(\infty) - \delta_l(0) = -\pi N_b. \tag{16.4}$$

We will now prove this important relation. Consider the function

$$D_l(k) = \chi_{kl}^{(+)}(0), \quad D_l^*(k) = (-1)^l D_l(-k). \tag{16.5}$$

$D_l(k)$ is analytic in the upper k halfplane; on the imaginary axis it has zeros corresponding to bound states. By (13.2) and (13.3) S_l can be written in the form

$$S_l(k) = \frac{D_l^*(k)}{D_l(k)} = (-1)^l \frac{D_l(-k)}{D_l(k)}. \tag{16.6}$$

As before, consider the integral

$$I = \int_{-\infty}^{\infty} \frac{S_l'(k)}{S_l(k)}\, dk = 4i\,(\delta_l(\infty) - \delta_l(0)).$$

Expressing S_l in terms of D_l and completing the contour in the upper half-plane, we obtain

$$I = -\int_{-\infty}^{\infty} \left[\frac{D'(-k)}{D(-k)} + \frac{D'(k)}{D(k)}\right] dk = -2\int_{-\infty}^{\infty} \frac{D'(k)}{D(k)}\, dk = -4\pi i N_b.$$

Comparison of the two expressions for I gives (16.4).

This proof of Levinson's theorem* is clearly applicable also if the total number of poles is finite. Comparison of (16.3) and (16.4) gives in this case

$$N_r = N_b + N_v + 2N_q. \tag{16.7}$$

We thus established the following remarkable fact: for potentials giving rise to a finite number of poles in the S-matrix, the number of redundant poles is completely determined by the number of bound, virtual, and quasistationary states. The simplest case $N_b = 1$, $N_v = N_q = 0$ ($N_v = 1$, $N_b = N_q = 0$) thus leads to a single redundant pole and corresponds to the "effective range approximation" /112, 132/ $\left(k \cot \delta = -\frac{1}{a} + \frac{1}{2} r_0 k^2 \text{ for } r_0 > 0\right)$.

We can now proceed with the derivation of the general dispersion relations for $S_l(k)$. We know that $S_a(k) = e^{2ika} S(k)$ is analytic in the upper k halfplane.

Consider the integral

$$\int_{-\infty}^{\infty} \frac{g_a(k)}{(k-z)k}\, dk, \quad g_a(k) = S_a^{-1}(k), \tag{16.8}$$

where z is some point in the first quadrant of the k plane. Completing the contour in the upper halfplane and noting that integration along the semicircle gives a zero contribution, we can write that this integral is equal to

$$2\pi i \times (\text{sum of residues in the upper halfplane}) =$$

$$= 2\pi i \left\{\frac{g_a(z)}{z} + \sum_n \frac{\operatorname{Res} g_a(k)}{(k-z)k}\Big|_{k=k_n}\right\}. \tag{16.9}$$

Here the first term corresponds to the pole at $k = z$ and the sum corresponds to bound states. Let now the imaginary part of z approach zero, so that z approaches a point z_0 on the real axis (Figure 10). Clearly

$$\int_{-\infty}^{\infty} \frac{g_a(k)\, dk}{(k-z)k} = \mathrm{P}\int_{-\infty}^{\infty} \frac{g_a(k)\, dk}{k(k-z_0)} + \pi i \frac{g_a(z_0)}{z_0},$$

* Another fairly simple derivation of Levinson's theorem can be found in /127/. Note that this theorem can be extended to a more general class of Hamiltonians /128/. A generalization of Levinson's theorem was derived in /129, 130/. Finally, in /131/ this theorem was proved for the relativistic case.

where P signifies that the integral is to be taken in the sense of its principal value. Equating this expression to (16.9), where we should also take the limit $z \to z_0$, we finally obtain /104/

$$\frac{g_a(z_0)}{z_0} = \frac{1}{\pi i} \mathrm{P} \int_{-\infty}^{\infty} \frac{g_a(k)\,dk}{(k - z_0)\,k} - 2 \sum_n \frac{\operatorname{Res} g_a(k_n)}{k_n (k_n - z_0)}.$$

Using (15.3) we write this so-called dispersion relation for $g_a(z_0)$ in the form

$$\frac{g_a(z_0)}{z_0} = \frac{1}{\pi i} \mathrm{P} \int_{-\infty}^{\infty} \frac{g_a(k)}{(k - z_0)k}\,dk - 2i \sum_n \frac{(-1)^{l+1} e^{-a|k_n|a} |A_n|^2}{k_n (k_n - z_0)}, \tag{16.10}$$

where A_n is the coefficient before $e^{-|k_n|r}$ in the normalized wave function of the bound state. The sum, as is clear from the derivation, is extended over all the bound states which exist for the given orbital momentum value.

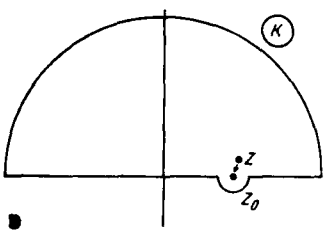

FIGURE 10.

Having derived expression (16.10), we can write without much difficulty an analogous expression for $f_a(k, \theta) = e^{2ika \sin \frac{\theta}{2}} f(k, \theta)$, where f is the scattering amplitude,

$$f(k, \theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l + 1)\,(S_l(k) - 1)\,P_l(\cos\theta).$$

This dispersion relation has the form

$$f_a(k, \theta) = \frac{1}{\pi i} \mathrm{P} \int_{-\infty}^{\infty} \frac{f_a(k', \theta)}{k' - k}\,dk' - \sum_{n, l} (2l + 1)\,P_l(\cos\theta) \frac{(-1)^{l+1} |A_{nl}|^2 e^{-a|k_{nl}| a \sin \frac{\theta}{2}}}{k_{nl}(k_{nl} - k)}. \tag{16.11}$$

Here the sum in the second term is taken over all the bound states of the system: over all values of the orbital momentum l for which bound states exist and over all states (the index n) for fixed l.

The above formula can be rewritten in a somewhat different form if we use the relation

$$f_a(-k, \theta) = f_a^*(k, \theta).$$

Then (16.7) takes the form

$$f_a(k,\theta)=\frac{1}{\pi i}\,\mathrm{P}\int_0^\infty dk'\left[\frac{f_a(k',\theta)}{k'-k}-\frac{f_a^*(k',\theta)}{k'+k}\right]-$$

$$-\sum_{nl}(2l+1)\,P_l(\cos\theta)\,\frac{|A_{nl}|^2(-1)^{l+1}e^{-a|k_{nl}|\sin\frac{\theta}{2}}}{k_{nl}(k_{nl}-k)}. \qquad (16.12)$$

The advantages of this expression are that the integration is carried out only over the physically meaningful positive values of the wave vector.

Dispersion relations which follow from the analyticity of $S_l(k)$ in the upper halfplane impose fairly rigid constraints on the energy dependence of these functions and on the energy dependence of the scattering amplitude. In particular, as we see from (16.12), they permit reconstructing the real (imaginary) part of f_a if we know its imaginary (real) part and the position and the coefficients A_{nl} of all the bound states. The dispersion relation for zero angle $\theta = 0$ is of particular importance, since in this case the dependence on the interaction range drops out and the amplitude $f(k, 0)$ can be expressed entirely in terms of experimentally observed quantities. To prove this point, we return to the optical theorem of the previous chapter

$$\mathrm{Im}\,f(k,0)=\frac{k}{4\pi}\sigma(k),$$

where $\sigma(k)$ is the total cross section. Using the optical theorem and dispersion relation (16.12) for $\theta = 0$, the real part of $f(k, 0)$ can be written in the form

$$\mathrm{Re}\,f(k,0)=\frac{1}{2\pi^2}\,\mathrm{P}\int_0^\infty dk'\,\frac{k'^2\sigma(k')}{k'^2-k^2}-\mathrm{Re}\sum_{l=0}^{\infty}(2l+1)\,\frac{(-1)^{l+1}|A_{nl}|^2}{k_{nl}(k_{nl}-k)}. \qquad (16.13)$$

This relation expresses the amplitude $f(k, 0)$ in terms of experimentally observed quantities:

$$f(k,0)=\mathrm{Re}\,f(k,0)+i\,\frac{k}{4\pi}\sigma(k), \qquad (16.14)$$

where the real part is given by (16.13).

Relations (16.10)—(16.14) were derived for the simplest case of potential scattering. However, analogous relations can be obtained for much more general assumptions concerning the particle interaction. Dispersion relations have a multitude of uses; for example, one of the main problems of nuclear physics and elementary particle physics is experimental determination of scattering phases, as they yield valuable information on the nature of particle interaction. Phase analysis (i.e., determination of the phases $\delta_l(k)$ from experimental cross section data for a fixed k), however, is not a single-valued procedure. This is particularly evident for the case of spinless particles: the cross section $\sigma(\theta, k)$ is readily seen to remain constant when the sign of all the phases is changed. This means that if we have found a range of phases which give a good fit between the theoretical and the experimental cross section $\sigma(\theta, k)$, the same fit can be obtained by changing the sign of all the phases. There is absolutely no possibility to determine the true sign of the phases $\delta_l(k)$ from the cross section $\sigma(\theta, k)$ at the same energy. This ambiguity is resolved only by

using the dispersion relation (16.13) which defines $f(k, 0)$ and thus gives the correct sign of the phases if the total cross section $\sigma(k)$ is known for all k and the parameters of the bound states are also given.

In conclusion note that in the derivation of the dispersion relations we only used the analyticity of $S_l(k)$ in the upper halfplane. No assumptions were made concerning the field acting on the particle. This is not accidental. The point is that irrespective of the actual potentials, any physical theory should satisfy the causality principle. This leads, as we have shown in § 13, to the analyticity of $S_l(k)$ in the upper halfplane and thus ensures the existence of dispersion relations. *

In deriving the dispersion relations, we always have to consider the convergence of the integrals at the upper limit. For example, the integral in (16.13) converges only if the total cross section for large k decreases faster than $1/k$, and this is not always so. Therefore we are generally dealing with dispersion relations not for amplitudes but for some functions with better convergence. Good convergence is ensured, say, by the ratio $\frac{f(k, \theta)}{(k+\alpha)^n}$ or by the difference $f(k, \theta) - f_{\text{Born}}(k, \theta)$, where $f_{\text{Born}}(k, \theta)$ is the amplitude computed in the Born approximation. The results of the next chapter show that this approximation is quite adequate for $k \to \infty$, so that the last difference rapidly converges for large k.

* This problem is treated in some detail in /104–106/.

Chapter 4

GREEN'S FUNCTION AND PERTURBATION THEORY

§ 17. INTRODUCTION. GREEN'S FUNCTION OF THE RADIAL SCHROEDINGER EQUATION

We have so far dealt only with the homogeneous Sch. Eq. In some problems, however, we have to solve the inhomogeneous Sch. Eq. Two very important classes of problems are in fact reduced to inhomogeneous equations.

First, these are the problems of perturbation theory, when we are looking for corrections to the wave function associated with small perturbations of the system Hamiltonian. The inhomogeneous term in the Sch. Eq. is proportional to the unperturbed wave function. Second, these are problems associated with reactions, i.e., with particle creation. Inhomogeneity in these problems plays the part of a source (or a sink) of new particles.

Handling of inhomogeneous equations requires thorough knowledge of the apparatus of Green's functions. Note that this apparatus is also applicable to the solution of equations which are much more involved than the Sch. Eq. (e.g., the equations of quantum field theory), and it is currently used on a very large scale almost in all subdivisions of theoretical physics.

We will only consider Green's functions of the Sch. Eq. The simplest of these is Green's function of the radial Sch. Eq., which is discussed in § 17. In § 18 and § 19 we consider some properties of Green's function of the three-dimensional Sch. Eq. In § 20 an expression is given for Green's function of several free particles. Then we pass on to a discussion of perturbation theory. In § 21 and § 22 we consider the application of perturbation theory in the coordinate and momentum representation. The next section gives simple examples illustrating when the perturbation theory is inapplicable and the entire perturbation-theoretical series must be summed.

The Feynman diagram technique, which presents a graphic picture of the structure of perturbation theoretical series, is derived for some particular simple cases in § 24. The last section (§ 25) of this chapter investigates the properties of the time-dependent Green's function.

The inhomogeneous Sch. Eq. is written in the form

$$\left(-\frac{\hbar^2}{2m}\Delta + U - E\right)\psi = -\frac{Q}{r}. \qquad (17.1)$$

Here Q is a function, called the source function or simply the source. The wave function ψ of this equation is subject to the usual conditions of single-valuedness and boundedness.

For a function satisfying (17.1) the probability density, in general, is not conservative. Indeed, the time-dependent equation equivalent to (17.1) has the form

$$i\hbar \frac{\partial \psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\Delta + U\right)\psi + \frac{Q}{r}e^{-\frac{iEt}{\hbar}}. \tag{17.1'}$$

We thus get in the usual way

$$i\hbar \frac{\partial}{\partial t}\int_V |\psi(r, t)|^2 dr = -\frac{\hbar^2}{2m}\int_S dS\,(\psi^*\nabla\psi - \psi\nabla\psi^*) + \int_V \left(\frac{Q}{r}e^{-\frac{iEt}{\hbar}}\psi^* - \frac{Q^*}{r}e^{\frac{iEt}{\hbar}}\psi\right) dr.$$

Separating the time, $\psi(r, t) = \psi(r)\, e^{-\frac{iEt}{\hbar}}$, we find that even in the stationary case the flux through a sphere of large radius does not vanish:

$$\int_S j\, dS = \frac{i}{\hbar}\int_V \left(\frac{Q^*}{r}\psi(r) - \frac{Q}{r}\psi^*(r)\right) dr.$$

Q is thus interpreted as a source or a sink of particles.

Equation (17.1) will be solved using the apparatus of Green's functions. The Green's function of the equation

$$L_r\chi_k(r) = \left[\frac{d^2}{dr^2} + (k^2 - V(r))\right]\chi_k(r) = 0 \tag{17.2}$$

is by definition a symmetric function of two variables $G_k(r, r')$ which satisfies the equation

$$L_r G_k(r, r') = \delta(r - r'). \tag{17.3}$$

The usefulness of this function is obvious. Indeed, using this function, we write the general solution of the inhomogeneous equation $L_r\varphi = Q$ in the form

$$\varphi_k(r) = \chi_k(r) + \int_0^\infty dr'\, G_k(r, r')\, Q(r'), \tag{17.4}$$

where $\chi_k(r)$ is the general solution of the homogeneous equation (17.2). That φ is indeed a solution of the inhomogeneous equation can be verified without difficulty:

$$L_r\varphi = L_r\chi + \int_0^\infty dr'\, Q(r')\, L_r G_k(r, r') = \int_0^\infty dr' Q(r')\delta(r - r') = Q.$$

According to a known theorem the general solution of an inhomogeneous equation is a sum of the general solution of the corresponding homogeneous equation and any particular solution of the inhomogeneous equation, so that (17.4) is in fact the general solution of the inhomogeneous equation when χ_k is interpreted as the general solution of the homogeneous equation (17.2) satisfying appropriate boundary conditions.

Let us now find the Green's function of equation (17.2). In our case, this is a fairly easy undertaking. Let $r \neq r'$, so that

$$L_r G(r, r') = L_{r'} G(r, r') = 0.$$

Since the Green's function is symmetric in relation to its arguments, it clearly has the form

$$G_k(r, r') = \begin{cases} \chi_k^{(1)}(r)\,\chi_k^{(2)}(r') & \text{for } r > r', \\ \chi_k^{(2)}(r)\,\chi_k^{(1)}(r') & \text{for } r < r', \end{cases} \tag{17.5}$$

where $\chi_k^{(1)}$ and $\chi_k^{(2)}$ are any two solutions of the homogeneous equation. For $r = r'$ (17.3) must be satisfied. This imposes additional restrictions on the choice of the functions $\chi^{(1)}$ and $\chi^{(2)}$. Indeed, condition (17.3) implies that

$$\int_{r-\Delta}^{r+\Delta} dr' L_r G_k(r, r') = 1 \tag{17.6}$$

for any arbitrarily small Δ. Let us evaluate this integral. If $\chi^{(1)} \neq \chi^{(2)}$, the function (17.5) is bounded and continuous, but its derivative is discontinuous at $r = r'$. This signifies that $(k^2 - V)\,G_k$ is bounded and integration over an infinitesimal neighborhood of r gives a zero contribution in (17.6). Relation (17.6) thus can be rewritten in the form

$$\int_{r-\Delta}^{r+\Delta} dr' \frac{d^2}{dr^2} G_k(r, r') = 1. \tag{17.6'}$$

We compute the first derivative:

$$\frac{d}{dr} G_k(r, r') = \begin{cases} \chi_k^{(1)\prime}(r)\,\chi_k^{(2)}(r') \to \chi_k^{(1)\prime}(r)\,\chi_k^{(2)}(r), \\ \quad r > r' \qquad\quad r' \to r \\ \chi_k^{(2)\prime}(r)\,\chi_k^{(1)}(r') \to \chi_k^{(1)}(r)\,\chi_k^{(2)\prime}(r). \\ \quad r < r' \qquad\quad r' \to r \end{cases} \tag{17.7}$$

It is discontinuous at the point $r = r'$ and is thus a step function. The second derivative $\frac{d^2}{dr^2} G_k(r, r')$ is therefore infinite at $r = r'$. The integral in (17.6) is clearly equal to

$$\int_{r-\Delta}^{r+\Delta} dr' \frac{d^2}{dr^2} G_k(r, r') = \chi_k^{(1)\prime}(r)\,\chi_k^{(2)}(r) - \chi_k^{(1)}(r)\,\chi_k^{(2)\prime}(r).$$

Function (17.5) is thus Green's function if

$$\chi_k^{(1)\prime}(r)\,\chi_k^{(2)}(r) - \chi_k^{(1)}(r)\,\chi_k^{(2)\prime}(r) = 1. \tag{17.8}$$

This condition is met by two pairs of solutions having the asymptotic expressions*

$$\chi_k^{(1)} \sim -e^{\pm i\left(kr - \frac{\pi l}{2} + \delta_l\right)}, \quad \chi_k^{(2)} \sim \frac{1}{k} \sin\left(kr - \frac{\pi l}{2} + \delta_l\right). \tag{17.9}$$

* We take the potential in the form $V(r) = V_0(r) + \frac{l(l+1)}{r^2}$.

Inserting these functions in the Wronskian (17.8), we readily see that it is equal to unity at infinity, where the above asymptotic expressions apply. Since the Wronskian is independent of r, (17.8) is valid for all r.

Thus, two Green's functions of the homogeneous equation have the form

$$G_{kl}^{(\pm)}(r, r') = -\sqrt{\frac{\pi}{2}}\frac{1}{k}\chi_{kl}^{(\pm)}(r_>)\chi_{kl}(r_<), \tag{17.10}$$

where $r_>$ and $r_<$ are respectively the larger and the smaller of the two radii r and r'; the functions $\chi_{kl}^{(\pm)}$ and χ_{kl} are defined by their asymptotic expressions

$$\chi_{kl}^{(\pm)}(r) \underset{r\to\infty}{\sim} e^{\pm i\left(kr-\frac{\pi l}{2}+\delta_l\right)}; \quad \chi_{kl}(r) \underset{r\to\infty}{\sim} \sqrt{\frac{2}{\pi}}\sin\left(kr-\frac{\pi l}{2}+\delta_l\right).$$

Corresponding to these two Green's functions we have two independent solutions of the inhomogeneous equation

$$\varphi_{kl}^{(\pm)} = \int_0^\infty dr'\, G_{kl}^{(\pm)}(r, r')\, Q(r') = \\ -\sqrt{\frac{\pi}{2}}\frac{1}{k}\left\{\chi_{kl}^{(\pm)}(r)\int_0^r dr'\chi_{kl}(r')\, Q(r') + \chi_{kl}(r)\int_r^\infty dr'\,\chi_{kl}^{(\pm)}(r')\, Q(r')\right\}. \tag{17.11}$$

First, direct substitution will show that these functions indeed solve the inhomogeneous equation. Since χ_{kl} and $\chi_{kl}^{(\pm)}$ behave for $r \to 0$ as r^{l+1} and r^{-l}, respectively, $\varphi_{kl}^{(\pm)}$ are regular at the origin if $Q(r)$ increases for $r \to 0$ not faster than $1/r^3$. At infinity the second term in (17.11) approaches zero (if, as is usually the case, $Q(r)$ falls off sufficiently fast with increasing r) and $\varphi_{kl}^{(\pm)}$ has the form of an incoming or an outgoing wave:

$$\varphi_{kl}^{(\pm)}(r) \underset{r\to\infty}{\sim} -\sqrt{\frac{\pi}{2}}\frac{1}{k}e^{\pm i\left(kr-\frac{\pi l}{2}+\delta_l\right)}\int_0^\infty dr\;\chi_{kl}(r')\, Q(r'). \tag{17.12}$$

Note that besides $G_{kl}^{(\pm)}$, one can construct various other Green's functions. We will not consider these alternatives, however, as they are either linear combinations of the functions $G^{(\pm)}$ or generate solutions of the inhomogeneous equation which do not satisfy the boundary condition for $r \to 0$.

The most general solution of the inhomogeneous equation can be now written in the form

$$\beta\chi_{kl}(r) + \alpha\varphi_{kl}^{(+)}(r) + (1-\alpha)\,\varphi_{kl}^{(-)}(r), \tag{17.13}$$

where α and β are arbitrary constants. The amplitudes of the incoming and the outgoing currents, in general, are not equal on account of the second and the third term. In other words, the inhomogeneity Q in the Sch. Eq. corresponds, as we have already noted, to introduction into our physical problem of a mechanism which is responsible for absorption or emission of particles. It should be stressed that for a given source Q the creation (or absorption) probability may vary between wide limits. It is entirely determined by the boundary conditions at infinity, i.e., by the values of the constants α and β.

For negative energies, the ordinary Sch. Eq., as we know, may have solutions which satisfy the boundary conditions only for some discrete

energy values. In the inhomogeneous Sch. Eq. the situation is different: for any energy E we always have a bounded solution $\varphi_{kl}^{(+)}$ which vanishes for $r \to 0$. That the solution is regular at the origin is proved in the paragraph following equation (17.11). That $\varphi_{kl}^{(+)}$ is regular at infinity follows from (17.12), where we should put $k = i|k|$. Notice that the particle current at negative energies is identically zero since the wave function ($\varphi^{(+)} \sim e^{-|k|r}$) in this case is real. It describes particles localized in space around the source; these particles cannot escape to infinity for lack of energy. However, for E which is equal to an eigenvalue of the homogeneous equation, the solution $\varphi^{(+)}$ does not exist whenever Q is not orthogonal to the bound-state wave function.

Indeed, let E_n be the energy of a bound state, and φ_n and φ solutions of the homogeneous and the inhomogeneous equation, respectively:

$$\varphi'' + \frac{2m}{\hbar^2}(E_n - U)\varphi = Q, \quad \varphi_n'' + \frac{2m}{\hbar^2}(E_n - U)\varphi_n = 0.$$

Multiplying the first equation by φ_n, the second by φ, and subtracting, we integrate the two sides of the equality over r from zero to R. Seeing that both solutions are regular for $r \to 0$, we find

$$\varphi'\varphi_n - \varphi\varphi_n'\Big|_{r=R} = \int_0^R Q(r')\varphi_n(r')\,dr'.$$

For $R \to \infty$ the solution φ should remain bounded and φ_n should decrease exponentially; the left-hand side therefore vanishes for $R \to \infty$. Thus, if φ exists, we inevitably come to the condition

$$\int_0^\infty dr'\, Q(r')\varphi_n(r') = 0. \tag{17.14}$$

§ 18. A REGULAR METHOD OF DERIVING GREEN'S FUNCTIONS. GREEN'S FUNCTION OF THE THREE-DIMENSIONAL SCHROEDINGER EQUATION

In the previous section we derived an expression for the Green's function of the radial Sch. Eq. We used a typical "pedestrian" method. In more complex cases, such "pedestrian" methods are much too tedious and a better approach is to use a general algorithm for the construction of Green's functions.

The underlying idea of this technique is surprisingly simple. Consider a differential operator L. The eigenfunctions φ_ε satisfying the boundary condition constitute a complete system:

$$L_x\varphi_\varepsilon(x) = \varepsilon\varphi_\varepsilon(x); \quad \sum_\varepsilon \varphi_\varepsilon(x)\varphi_\varepsilon^*(x') = \delta(x - x'). \tag{18.1}$$

We now form a function

$$G(x, x') = \sum_\varepsilon \frac{\varphi_\varepsilon(x)\varphi_\varepsilon^*(x')}{\varepsilon}, \tag{18.2}$$

which is clearly a Green's function, since by (18.1)

$$L_x G(x, x') = \sum_\varepsilon \frac{L_x \varphi_\varepsilon(x) \varphi_\varepsilon^*(x')}{\varepsilon} = \sum_\varepsilon \varphi_\varepsilon(x) \varphi_\varepsilon^*(x') = \delta(x - x').$$

As an example, we apply this method to the three-dimensional Sch. Eq.

$$H\psi_E = \left(-\frac{\hbar^2}{2m}\Delta + U\right)\psi_E(\boldsymbol{r}) = E\psi_E(\boldsymbol{r}). \tag{18.3}$$

The complete set of orthonormal solutions of this equation, as we have shown in Chapter 2, comprises the functions of the discrete spectrum and the continuum:

$$\psi_{nlm}(\boldsymbol{r}) = \frac{\chi_{nl}(r)}{r} Y_{lm}\left(\frac{\boldsymbol{r}}{r}\right), \quad \psi_k^{(+)}(\boldsymbol{r}). \tag{18.3'}$$

We will now construct the Green's function of the equation

$$(H - E_0)\psi_{E_0}(\boldsymbol{r}) = \left(-\frac{\hbar^2}{2m}\Delta + U - E_0\right)\psi_{E_0}(\boldsymbol{r}) = 0, \tag{18.4}$$

where E_0 is some fixed energy $E_0 = \frac{\hbar^2 k_0^2}{2m}$.

According to the general prescription, we first find a complete set of eigenfunctions of the operator $H - E_0$. We start with the fact that the functions (18.3') constitute a complete set of solutions of the equation

$$(H - E_0)\psi_E = (E - E_0)\psi_E.$$

We now write

$$G_{E_0}^{(\pm)}(\boldsymbol{r}, \boldsymbol{r}') = -\frac{2m}{\hbar^2}\left\{\sum_{nlm} \frac{\psi_{nlm}(\boldsymbol{r})\psi_{nlm}^*(\boldsymbol{r}')}{k_0^2 - k_{nl}^2} + \int dk \frac{\psi_k^{(\pm)}(\boldsymbol{r})\psi_k^{(\pm)*}(\boldsymbol{r}')}{k_0^2 - k^2 \pm i\gamma}\right\}, \tag{18.5}$$

where γ is an infinitesimal positive number whose meaning will become clear from what follows; the summation is carried out over all the bound states. Inserting explicit expressions for $\psi_k^{(\pm)}$ and integrating over the angular variable, we find for the second term in braces

$$\sum_{lm} Y_{lm}\left(\frac{\boldsymbol{r}}{r}\right) Y_{lm}^*\left(\frac{\boldsymbol{r}'}{r'}\right) Q_{kl}^{(\pm)}(r, r') \frac{1}{rr'}, \tag{18.6}$$

where

$$Q_{kl}^{(\pm)}(r, r') = \int_0^\infty dk \frac{\chi_{kl}(r)\chi_{kl}^*(r')}{k_0^2 - k^2 \pm i\gamma}. \tag{18.7}$$

If r and r' are so large that χ can be replaced by their asymptotic expressions, the integral in (18.7) is readily calculated:

$$Q_{kl}^{(\pm)}(r, r') = -\frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{dk}{k_0^2 - k^2 \pm i\gamma}\{(-1)^l S_l(k) e^{ik(r+r')} - e^{ik(r-r')}\}.$$

The integrand is exponentially small in the upper k halfplane (for $r > r'$), and the integration contour can therefore be chosen as shown in Figures 11, 12. The value of the integral is entirely determined by the poles of the integrand in the upper k halfplane. These are the poles of $S(k)$ for $k = k_{nl}$, corresponding to bound states, and the poles of the denominator for $k = \pm \sqrt{k_0^2 \pm i\gamma}$.

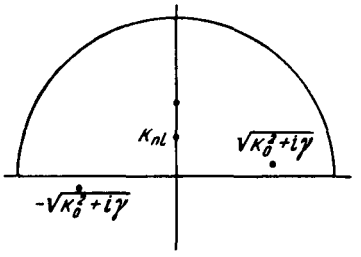

FIGURE 11.

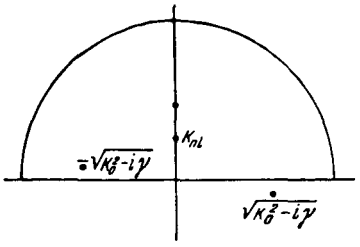

FIGURE 12.

For $Q^{(+)}$ the poles of the denominator are situated as shown in Figure 11, and the poles of $S(k)$ lie on the imaginary axis, so that for $r > r'$ the integral is equal to

$$Q_{k_0 l}^{(+)}(r, r') = -\frac{2\pi i}{2\pi}\left\{(-1)^l \sum_n \frac{e^{-|k_n|(r+r')}}{k_0^2 - k_n^2} \operatorname{Res} S_l(k)|_{k=k_n} - \right.$$
$$\left. - \frac{1}{2k_0}\left[(-1)^l S_l(k_0)\, e^{ik_0(r+r')} - e^{ik_0(r-r')}\right]\right\}. \qquad (18.8)$$

Hence for $G_{E_0}^{(+)}(r, r')$ for sufficiently large r and r' we have

$$G_{E_0}^{(+)}(r, r') = -\frac{2m}{\hbar^2}\sum_{lm} Y_{lm}\left(\frac{r}{r}\right) Y_{lm}^*\left(\frac{r'}{r'}\right)\frac{1}{rr'} \times$$
$$\times\left(-\frac{1}{k_0}\, e^{i\left(k_0 r_> - \frac{\pi l}{2} + \delta_l\right)} \sin\left(k_0 r_< - \frac{\pi l}{2} + \delta_l\right)\right). \qquad (18.9)$$

The first term in (18.8) canceled with the first term in (18.5) owing to the relation between the residue of $S(k)$ and the normalizing constant of the bound-state function (see § 15).

We know from the previous section that Green's function of the radial Sch. Eq. for large r and r' is

$$G_{kl}^{(+)}(r, r') = -\frac{1}{k} e^{i\left(kr_> - \frac{\pi l}{2} + \delta_l\right)} \sin\left(kr_< - \frac{\pi l}{2} + \delta_l\right).$$

Therefore (18.9) can be rewritten as

$$G_{E_0}^{(+)}(r, r') = -\frac{2m}{\hbar^2}\sum_{lm}\frac{1}{rr'} G_{k_0 l}^{(+)}(r, r') Y_{lm}\left(\frac{r}{r}\right) Y_{lm}^*\left(\frac{r'}{r'}\right). \qquad (18.10)$$

It is readily verified that this formula for Green's function is valid for all r and r' if for $G_{k_0 l}^{(\pm)}(r, r')$ we use the exact expression (17.10). Indeed,

inserting (18.10) in the Sch. Eq. we find

$$\frac{\hbar^2}{2m}\left[-\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{\hat{L}^2}{r^2}+V-k_0^2\right]G_{E_0}^{(+)}(r,r')=$$
$$=-\sum_{lm}Y_{lm}\left(\frac{r}{r}\right)Y_{lm}^*\left(\frac{r'}{r'}\right)\frac{1}{rr'}\left[-\frac{d^2}{dr^2}+V+\frac{l(l+1)}{r^2}-k_0^2\right]\times$$
$$\times G_{k_0}^{(+)}(r,r')=\sum_{lm}Y_{lm}\left(\frac{r}{r}\right)Y_{lm}^*\left(\frac{r'}{r}\right)\frac{1}{r^2}\delta(r-r')=\delta(r-r').$$

Here $\hat{L}^2$ is the operator of the square of the orbital momentum:

$$\hat{L}^2Y_{lm}=-\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]Y_{lm}=l(l+1)Y_{lm}.$$

Moreover we used the obvious equality which follows from the completeness property of the spherical functions Y_{lm}:

$$\sum_{lm}Y_{lm}(\theta,\varphi)Y_{lm}^*(\theta',\varphi')=\delta(\cos\theta-\cos\theta')\,\delta(\varphi-\varphi'),$$

where θ, θ', φ, φ' are the polar and the azimuthal angles of the vectors $\frac{r}{r}$, $\frac{r'}{r'}$.

If we take the minus sign before γ in the denominator of (18.5) the corresponding position of the poles of the integrand is shown in Figure 12.

Proceeding along the same lines as before, we get

$$G_{E_0}^{(-)}(r,r')=-\frac{2m}{\hbar^2}\sum\frac{1}{rr'}G_{k_0}^{(-)}(r,r')\,Y_{lm}\left(\frac{r}{r}\right)Y_{lm}^*\left(\frac{r'}{r'}\right). \tag{18.11}$$

Clearly

$$G_{E_0}^{(-)}=G_{E_0}^{(+)*}. \tag{18.5'}$$

This, however, is also apparent from the general expression (18.5).

Using (18.10) and (18.11) we write the general solution of the inhomogeneous Sch. Eq.

$$\left(-\frac{\hbar^2}{2m}\Delta+U-E_0\right)\psi(r)=Q(r)$$

in the form

$$\psi^{(\pm)}(r)=\psi_{E_0}(r)+\int dr'\,G_{E_0}^{(\pm)}(r,r')\,Q(r'), \tag{18.12}$$

where $\psi_{E_0}(r)$ is the general solution of the homogeneous equation.

For large r Green's function can be written as

$$G_{E_0}^{(\pm)}(r,r')\sim\frac{2m}{\hbar^2}\sqrt{\frac{\pi}{2}}\frac{1}{k_0}\sum_{lm}Y_{lm}\left(\frac{r}{r}\right)Y_{lm}^*\left(\frac{r'}{r'}\right)\frac{1}{rr'}\times$$
$$\times e^{\pm i\left(k_0r-\frac{\pi l}{2}+\delta_l\right)}\chi_{k_0l}(r')=\frac{2m}{\hbar^2}\frac{e^{\pm ik_0r}}{r}\psi_{\pm k_0\frac{r}{r}}^{(\mp)*}(r'). \tag{18.13}$$

In the derivation we made use of the known properties of spherical harmonics and of the definition of orthonormal continuum functions $\psi_k^{(\pm)}(r)$ (see § 10, § 11).

From (18.13) we see that the solution of the inhomogeneous equations behaves asymptotically as

$$\psi^{(\pm)}(r)\underset{r\to\infty}{\sim}\psi_{E_0}(r)+\frac{2m}{\hbar^2}\frac{e^{\pm ik_0 r}}{r}\int dr'\,Q(r')\,\psi^{(\mp)*}_{\pm k_0\frac{r}{r}}(r'), \tag{18.14}$$

i.e., inhomogeneity gives rise to incoming or outgoing particle currents, so that, as with the radial equation, it can be interpreted as a source (or a sink) of particles.

The meaning of the infinitesimal constant γ introduced at the beginning of this section is now quite clear. If it enters (18.5) with the plus sign, we obtain the function $G^{(+)}$ which generates solutions corresponding to outgoing waves. If γ is preceded by minus sign, we obtain the complex conjugate function $G^{(-)}$ which corresponds to incoming wave solution.

In some very simple cases closed expressions for Green's function can be derived. For a free particle ($U = 0$), the Green's function is

$$G_E^{(\pm)}(r, r') = \frac{2m}{\hbar^2}\frac{1}{4\pi}\frac{e^{\pm ik|r-r'|}}{|r-r'|}. \tag{18.15}$$

In case of a Coulomb potential $U = -\frac{\alpha}{r}$, the explicit form of the Green's function was derived in /133/. A simpler method of derivation of this Green's function will be found in /134/. We give here only the final result:

$$G_E^{(c)(\pm)}(r, r') = G_{E\pm i\gamma}^{(c)}(r, r') = \frac{2m}{\hbar^2}\frac{\Gamma(1-i\eta)}{4\pi|r-r'|}\times$$
$$\times\frac{1}{ik}\left(-\frac{\partial}{\partial y}+\frac{\partial}{\partial x}\right)W_{i\eta;\,\frac{1}{2}}(-ikx)\,M_{i\eta;\,\frac{1}{2}}(-iky). \tag{18.16}$$

Here $\eta = \frac{m\alpha}{\hbar^2 k}$, $k = \sqrt{\frac{2mE}{\hbar^2}}$, $x = r + r' + |r - r'|$, $y = r + r' - |r - r'|$; $W_{i\eta;\,\frac{1}{2}}$ and $M_{i\eta;\,\frac{1}{2}}$ are known Whittaker's functions.

For $r' = 0$ the expression for Green's function takes the simpler form

$$G_E^{(c)(\pm)}(r, 0) = \frac{2m}{\hbar^2}\frac{1}{4\pi r}\Gamma(1-i\eta)\,W_{i\eta;\,\frac{1}{2}}(-2ikr). \tag{18.17}$$

This expression was first derived in /135/.

Note, however, that the Green's function of the Coulomb potential takes on its simplest form in the momentum representation if the invariance of the Sch. Eq. under four-dimensional rotations (for $E < 0$) /46/ or Lorentz transformations (for $E > 0$) /47/ is taken into consideration. In this case, it is convenient to introduce the function

$$G(\xi, \xi') = -\frac{1}{16mk^3}(p^2 \pm k^2)^2\,G_E(p, p')\,(p'^2 \pm k^2)^2. \tag{18.18}$$

The upper (lower) sign in this formula corresponds to $E < 0$ ($E > 0$) and the unit four-dimensional vector ξ has the form

$$\xi = \frac{2kp}{p^2 \pm k^2}, \quad \xi_0 = \frac{k^2 \mp p^2}{p^2 \pm k^2}. \tag{18.19}$$

Schwinger /46/ showed that for $E<0$, $G(\xi, \xi')$ can be written in the form

$$G(\xi, \xi') = \sum_{n=1}^{\infty} \sum_{l=0}^{n-1} \sum_{m=-l}^{l} \frac{Y_{nlm}(\xi) Y^*_{nlm}(\xi')}{1+\frac{\eta}{n}}, \tag{18.20}$$

where $Y_{nlm}(\xi)$ are the four-dimensional spherical functions. Carrying out the summation over l and m, we get

$$\begin{gathered} G(\xi, \xi') = \delta(\xi-\xi') - \frac{\eta}{2\pi^2(\xi-\xi')^2} + \frac{\eta^2}{4\pi^2 i} \frac{1}{\sin\chi} [\Phi(e^{i\chi}, \eta) - \Phi(e^{-i\chi}, \eta)], \\ \Phi(z, \eta) = \sum_{n=0}^{\infty} \frac{z^n}{n+\eta}, \quad (\xi, \xi') = \cos\chi. \end{gathered} \tag{18.21}$$

The expression for $G(\xi, \xi')$ for $E>0$ was derived in /47/:

$$G^{(\pm)}(\xi, \xi') = \int d\rho\, g_{ij}(\rho) \sum_{lm} Y_{\rho lm}(\xi) Y^*_{\rho lm}(\xi'), \tag{18.22}$$

$$\left.\begin{aligned} g^{(\pm)}_{11}(\rho) &= \left(1 - \frac{2\eta}{\rho} \operatorname{cth} \frac{\pi\rho}{2}\right) \frac{\rho^2/4}{\rho^2/4 - \eta^2 \pm i\gamma}, \\ g^{(\pm)}_{12}(\rho) &= g^{(\pm)}_{21}(\rho) = \frac{2\eta}{\rho \operatorname{sh} \frac{\pi\rho}{2}} \frac{\rho^2/4}{\rho^2/4 - \eta^2 \pm i\gamma}, \\ g^{(\pm)}_{22}(\rho) &= -\left(1 + \frac{2\eta}{\rho} \operatorname{cth} \frac{\pi\rho}{2}\right) \frac{\rho^2/4}{\rho^2/4 - \eta^2 \pm i\gamma}. \end{aligned}\right\}, \tag{18.23}$$

Here the functions $Y_{\rho lm}$ are analogous to the spherical functions for a two-sheet hyperboloid $\xi_0^2 - \boldsymbol{\xi}^2 = 1$ and the subscripts i, j mark the position of the tips of the vectors ξ and ξ' on the hyperboloid sheets: $i = 1\,(2)$ if ξ lies on the upper (lower) sheet; the subscript j similarly signifies the position of ξ'.

§ 19. SOME PROPERTIES OF GREEN'S FUNCTION

As we have shown in the previous section, the Green's function of the three-dimensional Sch. Eq. is expressed in terms of the Green's function of the radial equation. We will therefore concentrate on the latter only.

Consider the function

$$G^{(+)}_{k_0 l}(r, r') = -\sqrt{\frac{\pi}{2}} \frac{1}{k} \chi^{(+)}_{k_0 l}(r_>) \chi_{k_0 l}(r_<).$$

We see that $G^{(+)}_{k_0 l}$ is an analytic function of k_0 in the entire upper halfplane, except at the isolated points $k = k_{nl}$ on the imaginary axis (bound states), where it has poles. Near the poles, for large r and r' it behaves as

$$G^{(+)}_{kl}(r, r') \underset{k \to k_{nl}}{\to} -\frac{1}{k_{nl}} \frac{(-1)^l}{2i} e^{2i\delta_l(k)} e^{-|k_{nl}|(r+r')} = \frac{1}{2k_{nl}} \frac{1}{k-k_{nl}} |A_{nl}|^2 e^{-|k_{nl}|(r+r')}.$$

This expression suggests that for any r and r' we should take

$$G^{(+)}_{kl}(r, r') \underset{k \to k_{nl}}{\to} \frac{1}{2k_{nl}} \frac{\chi_{nl}(r) \chi^*_{nl}(r')}{k-k_{nl}} = \frac{\chi_{nl}(r) \chi^*_{nl}(r')}{k^2 - k^2_{nl}}, \tag{19.1}$$

where χ_{nl} is the normalized wave function of the n-th bound state. This expression is indeed always applicable. Except for the poles at the points $k = k_{nl}$, the Green's function has no other singularities in the upper k halfplane. For $|k| \to \infty$ and $r > r'$ it falls off exponentially. This is immediately obvious from the asymptotic expression

$$G_{kl}^{(+)}(r, r') \underset{|k|\to\infty}{\to} -\frac{1}{k}\frac{1}{2i}\left(e^{ik(r+r')}(-1)^l S_l(k) - e^{ik(r-r')}\right),$$

where we should put $k = k_1 + ik_2$ ($k_2 > 0$); this expression also shows that in the lower k halfplane the function $G^{(+)}$ is exponentially divergent for $|k| \to \infty$ and its poles coincide with the poles of $S_l(k)$. In the following we will show that the poles of $S_l(k)$ in the lower halfplane correspond to the so-called quasistationary states.

Thus, the poles of $G_{kl}^{(+)}$ in the upper halfplane correspond to stationary states, and those in the lower halfplane to quasistationary states.

Some important theorems can be proved using the integral representation of Green's function

$$G_{kl}^{(+)}(r, r') = \sum_n \frac{\chi_{nl}(r)\,\chi_{nl}^*(r')}{k^2 - k_n^2 + i\gamma} + \int_0^\infty dk' \frac{\chi_{k'l}(r)\,\chi_{k'l}^*(r')}{k^2 - k'^2 + i\gamma}. \tag{19.2}$$

Integration of (19.2) over k^2 yields

$$\int_{-\infty}^{\infty} dk^2 G_{kl}^{(+)}(r, r') = -\pi i\left\{\sum_n \chi_{nl}(r)\,\chi_{nl}^*(r') + \int_0^\infty dk' \chi_{k'l}(r)\,\chi_{k'l}^*(r')\right\} = -\pi i\delta(r - r'). \tag{19.3}$$

If we introduce a cutoff factor $C(k^2) \underset{k\to\infty}{\to} 0$, which is free from any singularities in the upper k^2 halfplane, e.g., $C_1(k^2) = e^{iak^2}$ with positive $a \to 0$, we find completing the integration contour in the upper halfplane

$$\int_{-\infty}^{\infty} G_{kl}^{(+)}(r, r') C_1(k^2)\, dk^2 = 0. \tag{19.4}$$

If the cutoff factor has no singularities in the lower halfplane, e.g.,

$$C_2(k^2) = e^{-iak^2},\ a > 0,$$

completing the contour in the lower halfplane we get

$$\int_{-\infty}^{\infty} dk^2 G_{kl}^{(+)}(r, r') C_2(k^2) = -2\pi i\delta(r - r'). \tag{19.5}$$

Representation (19.2) leads to still another interesting formula,

$$\int_0^\infty dr' G_{kl}^{(+)}(r, r')\,\chi_{k_1 l}(r') = \frac{\chi_{k_1 l}(r)}{k^2 - k_1^2 + i\gamma}, \tag{19.6}$$

whose proof only assumes that χ_{kl} are orthonormal functions.

We can similarly derive all the fundamental properties of the function $G_{kl}^{(-)}$. We will not go into this problem, however, as $G^{(-)}$ is hardly ever encountered in the applications.

The analytical properties of the Green's function of the three-dimensional Sch. Eq. constitute a trivial generalization of the corresponding properties of the radial Green's function. In particular, (19.3) and (19.6) are replaced by

$$\int_{-\infty}^{\infty} dE G_E^{(\pm)}(\boldsymbol{r}, \boldsymbol{r}') = \mp \pi i \delta(\boldsymbol{r} - \boldsymbol{r}'), \tag{19.3'}$$

$$\int d\boldsymbol{r}' G_E^{(\pm)}(\boldsymbol{r}, \boldsymbol{r}') \psi_p^{(\pm)}(\boldsymbol{r}') = -\frac{2m}{\hbar^2} \frac{\psi_p^{(\pm)}(\boldsymbol{r})}{k^2 - p^2 \pm i\gamma}. \tag{19.6'}$$

§ 20. GREEN'S FUNCTION FOR SEVERAL NONINTERACTING PARTICLES

Using the standard method, we can find Green's functions for the case of several noninteracting particles. For two particles, the Sch. Eq. has the form

$$(H_1 + H_2 - E)\psi_E = \left\{\left(-\frac{\hbar^2}{2m_1}\Delta_1 + U_1(\boldsymbol{r}_1)\right) + \right.$$
$$\left. + \left(-\frac{\hbar^2}{2m_2}\Delta_2 + U_2(\boldsymbol{r}_2)\right) - E\right\}\psi_E(\boldsymbol{r}_1, \boldsymbol{r}_2) = 0, \tag{20.1}$$

where $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ are the particle coordinates, m_1 and m_2 are the particle masses, U_1 and U_2 are the potentials that the particles see, and H_1 and H_2 are the corresponding Hamiltonians. As a complete set of functions of this equation we can take all the various products of the form $\psi_{k_1}(\boldsymbol{r}_1)\psi_{k_2}(\boldsymbol{r}_2)$ where ψ_{k_1}, ψ_{k_2} are the eigenfunctions of the Hamiltonians H_1 and H_2. Then forming an expression analogous to (18.5) and integrating, we easily find for Green's function

$$G_k^{(\pm)}(\boldsymbol{r}_1, \boldsymbol{r}_2;\ \boldsymbol{r}_1', \boldsymbol{r}_2') = \mp \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\varepsilon\, G_\varepsilon^{(\pm)}(\boldsymbol{r}_1, \boldsymbol{r}_1')\, G_{E-\varepsilon}^{(\pm)}(\boldsymbol{r}_2, \boldsymbol{r}_2'), \tag{20.2}$$

where $G_\varepsilon(\boldsymbol{r}_1, \boldsymbol{r}_1')$ and $G_{E-\varepsilon}(\boldsymbol{r}_2, \boldsymbol{r}_2')$ are Green's functions of the operators $(H_1 - \varepsilon)$ and $(H_2 - (E - \varepsilon))$, respectively. To check this expression, we act on the right-hand side with the operator $(H_1 + H_2 - E)$. Using the relations of the preceding section, we get

$$\mp \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\varepsilon [(H_1 - \varepsilon) + (H_2 - (E - \varepsilon))] G_\varepsilon^{(\pm)}(\boldsymbol{r}_1, \boldsymbol{r}_1')\, G_{E-\varepsilon}^{(\pm)}(\boldsymbol{r}_2, \boldsymbol{r}_2') =$$
$$= \mp \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\varepsilon \{\delta(\boldsymbol{r}_1 - \boldsymbol{r}_1')\, G_{E-\varepsilon}^{(\pm)}(\boldsymbol{r}_2, \boldsymbol{r}_2') +$$
$$+ \delta(\boldsymbol{r}_2 - \boldsymbol{r}_2') G_\varepsilon^{(\pm)}(\boldsymbol{r}_1, \boldsymbol{r}_1')\} = \delta(\boldsymbol{r}_1 - \boldsymbol{r}_1')\delta(\boldsymbol{r}_2 - \boldsymbol{r}_2'), \tag{20.3}$$

i.e., the right-hand side of (20.2) is indeed Green's function of equation (20.1).

We can similarly treat the case of three and more particles. In the general case of N noninteracting particles, the Sch. Eq. has the form

$$\left(\sum_{i=1}^{N} H_i - E\right)\psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) = 0, \tag{20.4}$$

and for Green's function we readily find

$$\begin{aligned} G_E^{(\pm)}(\mathbf{r}_1, \ldots, \mathbf{r}_N; \mathbf{r}'_1, \ldots, \mathbf{r}'_N) = \\ = \frac{1}{N}\frac{1}{(\mp\pi i)^{N-1}}\int_{-\infty}^{\infty} d\varepsilon_1 \ldots d\varepsilon_{N-1} G_{\varepsilon_1}^{(\pm)}(\mathbf{r}_1, \mathbf{r}'_1)\, G_{\varepsilon_1}^{(\pm)}(\mathbf{r}_1, \mathbf{r}'_1)\cdots \\ \cdots G_{\varepsilon_{N-1}}^{(\pm)}(\mathbf{r}_{N-1}, \mathbf{r}'_{N-1})\, G^{(\pm)}_{E-\sum_{i=1}^{N-1}\varepsilon_i}(\mathbf{r}_N, \mathbf{r}'_N). \end{aligned} \tag{20.5}$$

Here the + and − signs correspond to the two cases when all the particles emerge from the center (+) or they all converge to the center (−).

A significant aspect in the application of (20.2) and (20.5) is the choice of the path around the poles of Green's function corresponding to bound states. The prescription here is very simple. Since in the derivation of these relations we use the integral properties of Green's function (19.3'), the path around the poles in (20.2)—(20.5) should be precisely the same as that in (19.3'). In other words, the integration over ε should be carried out along the real axis and the position of the poles of Green's functions entering the integrand is automatically fixed by the sign of the infinitesimal constant γ in (18.5). In practice this means that when integrating $G_E^{(+)}$ we should replace E by $E_1 + i\delta$ ($\delta > 0$) and carry out the integration over E_1, and when integrating $G_E^{(-)}$ we should replace E by $E_1 - i\delta$.

To complete our brief survey of the properties of Green's functions, let us consider their behavior for close values of the arguments. We have seen in the preceding that the one-dimensional (radial) Green's function $G_{kl}(r, r')$ remains bounded for $r = r'$, whereas its derivative with respect to r or r' is discontinuous at this point. Green's function $G_E(\mathbf{r}, \mathbf{r}')$ of the three-dimensional Sch. Eq. for $\mathbf{r} = \mathbf{r}'$ goes to infinity at $\mathbf{r} = \mathbf{r}'$ as $\frac{2m}{\hbar^2}\frac{1}{4\pi}\frac{1}{|\mathbf{r}-\mathbf{r}'|}$. This is obvious from the following considerations: each term in (18.10) remains finite for $\mathbf{r} = \mathbf{r}'$. Therefore, any singularity of the function may be associated only with the weak convergence of the series (18.10) for large l. On the other hand, as we will see in the next section, the wave functions χ_{kl} in a potential $U(r)$ approach the free-particle functions for large l:

$$\chi_{kl}(r) \underset{l\to\infty}{\sim} \sqrt{\frac{2}{\pi}}\sin\left(kr - \frac{\pi l}{2}\right).$$

Therefore the radial Green's function also approaches the Green's function $\bar{G}_{kl}^{(\pm)}(r, r')$ of the Sch. Eq. with zero potential:

$$G_{kl}^{(\pm)}(r, r') \underset{l\to\infty}{\sim} -\frac{1}{k}e^{\pm\left(kr_> - \frac{\pi l}{2}\right)}\sin\left(kr_< - \frac{\pi l}{2}\right) \equiv \bar{G}_{kl}^{(\pm)}(r, r'). \tag{20.6}$$

Thus, $G(\mathbf{r}, \mathbf{r}')$ has the same singularity as in the case of a Sch. Eq. without a potential, when the Green's function can be found in explicit form:

$$\bar{G}_k^{(\pm)}(\mathbf{r}, \mathbf{r}') = -\frac{2m}{\hbar^2}\frac{1}{(2\pi)^3}\int d\mathbf{p}\frac{e^{i\mathbf{p}(\mathbf{r}-\mathbf{r}')}}{k^2 - p^2 \pm i\gamma} = \frac{2m}{\hbar^2}\frac{1}{4\pi}\frac{e^{\pm ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}.$$

This proves our assertion concerning the divergence of the three-dimensional Green's function for $r \to r'$. Hence it follows immediately that in all the physically relevant cases the difference

$$G_k^{(\pm)}(r, r') - \overline{G}_k^{(\pm)}(r, r')$$

is free from singularities at $r \to r'$ (except, of course, the singularities associated with bound states, when Green's function goes to infinity as a function of k for all r and r').

Similarly we can consider the many-particle Green's function (20.5). Its divergence for $r_i \to r_i'$ is also associated with large orbital momenta. However, the character of this divergence is different. For example, the two-particle Green's function (20.2) for equal arguments behaves as

$$\frac{1}{[(r_1 - r_1')^2 + (r_2 - r_2')^2]^2}.$$

§ 21. PERTURBATION THEORY: COORDINATE REPRESENTATION

The perturbation theory is probably the most popular and widely known topic of quantum mechanics.* The literature on the subject is very extensive, and we will therefore be as brief as possible. The problem is formulated as follows: let all the eigenfunctions $\psi_k^{(0)}$ and the eigenvalues of the Schroedinger equation

$$H_0 \psi_k^{(0)} = E \psi_k^{(0)} \tag{21.1}$$

be known. Find the corrections to the eigenfunctions and the eigenvalues which arise when the Hamiltonian H_0 is incremented by a small perturbation W. First we consider the scattering problem. The most general technique is to take the solution of the perturbed equation

$$(H_0 + W - E)\psi_k(r) = 0 \tag{21.2}$$

in the form

$$\psi_k = \psi_k^{(0)} + \varphi_k, \tag{21.3}$$

where the increment φ_k is assumed to be small. For φ_k we have the equation

$$(H_0 - E)\varphi_k = -W(\psi_k^{(0)} + \varphi_k). \tag{21.4}$$

Introducing Green's function $G_E(r, r')$ of the unperturbed operator $(H_0 - E)$, we write (21.4) as an integral equation

$$\varphi_k(r) = -\int dr' G_E(r, r') W(\psi_k^{(0)}(r') + \varphi_k(r')). \tag{21.5}$$

* There are several versions of the perturbation theory. The most commonly used is the Rayleigh–Schroedinger perturbation theory /136/; see also /137/. In this case both the wave function and the energy eigenvalue are series expanded in powers of a small parameter. Of the other variants we mention only the perturbation theory of Brillouin /138/ and Wigner /139/ (see also /140/), when only the wave function is series expanded.

Successive iterations of this equation give φ_k to any desired accuracy. To terms of second order in W, we have, say,

$$\varphi_k = -\int dr' G_E(r, r')\, W\psi_k^{(0)}(r') + \\ +\int dr' dr'' G_E(r, r')\, W G_E(r', r'')\, W\psi_k^{(0)}(r''). \qquad (21.6)$$

Any problem is thus reduced to the determination of Green's function G_E and the actual computation of the series (21.6). For an arbitrary Hamiltonian H_0, the Green's function has the form

$$G_E^{(+)}(r, r') = \sum_{nlm} \frac{\psi_{nlm}^{(0)}(r)\,\psi_{nlm}^{(0)*}(r')}{E - E_{nl}} + \int \frac{dp\psi_p^{(0)}(r)\,\psi_p^{(0)*}(r')}{E - E_p + i\gamma},$$

and to find it we need all the eigenfunctions and eigenvalues of the unperturbed level. This considerably complicates the computation of the series (21.6).

The position is essentially simplified, however, if we first consider potential scattering, i.e., an unperturbed Hamiltonian of the form

$$H_0 = -\frac{\hbar^2}{2m}\Delta + U(r).$$

We know from the previous sections that to find G_E we require only the solutions of the Sch. Eq. for the same energy value E (see (17.11) and (18.9)). The perturbation theoretical expressions are thus markedly simplified. To first order in the perturbation we have, assuming a spherically symmetric W,

$$\varphi_k(r) = \frac{2m}{\hbar^2}\frac{1}{kr}\sum_l i^l e^{i\delta_l}\sqrt{4\pi(2l+1)}Y_{l0}\left(\frac{kr}{kr}\right)\int_0^\infty dr' G_{kl}^{(+)}(r, r')\, W\chi_{kl}(r'). \qquad (21.7)$$

Here for $G_E(r, r')$ we used expression (18.10) and for $\psi_k^{(0)}$ the expression $\psi_k^{(0)} = \frac{1}{(2\pi)^{3/2}}e^{ikr}$.

In all the above formulas we have to use the Green's function $G^{(+)}$ corresponding to outgoing waves. This is readily seen from the following considerations. Incoming waves in the unperturbed function $\psi_k^{(0)}$ are determined by external conditions, namely by the current reaching the force center from infinity. This current is assumed to be known and independent of the interaction mechanism. Adding the perturbation W to the potential will thus only affect the outgoing waves. This in its turn means that we should use the function $G^{(+)}$ and not others.

The asymptotic behavior of φ for large r can be found from (18.13). This gives (to first order in the perturbation)

$$\varphi_k(r) \sim -\frac{e^{ikr}}{r}\frac{2m}{\hbar^2}\int dr' \psi_{kn}^{(0)(-)*}(r')\, W\psi_k^{(0)}(r'), \qquad (21.8)$$

where we introduced the unit vector $n = \frac{r}{r}$. Note that the final-state wave function in the matrix element is $\psi_{kn}^{(0)(-)}$. This is so, as we have mentioned

in the preceding, because these functions describe the wave of particles which are scattered in a definite direction (along the vector kn).

Using the expressions of this section, we can readily find the correction to the scattering amplitude due to the perturbation. * To first order in W, the scattering amplitude is

$$f(\theta) = \frac{1}{2ik} \sum_l \sqrt{4\pi(2l+1)}\, Y_{l0}\left(\frac{kr}{kr}\right)\left(e^{2i(\delta_l^{(0)}+\Delta\delta_l)} - 1\right). \tag{21.9}$$

Here $\delta_l^{(0)}$ is the unperturbed scattering phase, and

$$\Delta\delta_l = -\frac{\pi}{k}\frac{m}{\hbar^2}\int dr' \chi_{kl}^*(r')\, W \chi_{kl}(r'), \tag{21.10}$$

where $\chi_{kl}(r)$ are the radial functions of the unperturbed equation normalized to $\delta(k - k')$.

A necessary condition for the applicability of perturbation theory is $|\varphi_k| \ll |\psi^{(0)}|$.

If the perturbation W is localized within some volume V, the above relations apply

1) if $W \to 0$,

2) for any W, provided that $l \to \infty$ or $k \to \infty$.

The first condition is obvious. The second is associated with the smallness of the perturbation theoretical integrals in the two following cases:

(a) for $k \to \infty$ because the unperturbed wave functions widely oscillate;

(b) for $l \to \infty$ because the functions χ_{kl} are very small if the particle energy E is less than the centrifugal energy, i.e., when $r < \frac{l}{k}$.

We have thus laid the foundation for the treatment of the divergence of Green's functions for close values of the arguments given in the last section. The corresponding estimates are a trivial consequence of the above relations.

For discrete-spectrum functions the perturbation theoretical problem becomes more complicated, since besides wave function corrections, we should also find the corrections ΔE_{nl} for bound-state energies. The standard procedure of the perturbation theory in this case is well known, and we will not discuss it any further. We only note that finding the wave function corrections requires knowledge of all the eigenfunctions of the unperturbed equation. In case of a potential interaction, however, we can propose a method (as for the scattering problem), which uses the solutions of the unperturbed equation for one energy value only /147/.

The equation for the radial wave function now has the form

$$\chi_{nl}'' + \left(k_{nl}^2 - \frac{l(l+1)}{r^2} - V - w\right)\chi_{nl} = 0, \tag{21.11}$$

* An obvious shortcoming of the ordinary perturbation theory is that the scattering amplitude does not satisfy the unitarity condition. This led to the development of the so-called N/D method /141, 142/, which is free from this shortcoming. Comparison of numerical solutions obtained by this method with exact solutions is given in /143, 144/. Recently Dashen and Frautschi /145, 146/ developed a characteristic perturbation-theoretical method within the framework of the S-matrix formalism.

where $w = \frac{2m}{\hbar^2} W$, and k_{nl}^2 are related in the usual way to the new energy value of the bound state. The solution is sought in the form

$$\chi_{nl} = C_1(r)\,\chi_{nl}^{(0)}(r) + C_2(r)\,\varphi_{nl}^{(0)}(r), \tag{21.12}$$

where C_1 and C_2 are as yet unknown, and $\varphi_{nl}^{(0)}$ and $\chi_{nl}^{(0)}$ are respectively the irregular and the regular solutions of the unperturbed equation computed for the energy $E_0 = \frac{\hbar^2}{2m}(k_{nl}^{(0)})^2$ of the unperturbed bound state. The functions C_1 and C_2 are assumed to satisfy the condition

$$C_1'\chi_{nl}^{(0)} + C_2'\varphi_{nl}^{(0)} = 0. \tag{21.13}$$

In the theory of differential equation, this is known as the Lagrange condition. Inserting (21.12) in (21.11) and using (21.13) we obtain for C_1' and C_2' the exact equations

$$\left.\begin{aligned} C_1' &= -\frac{\varphi(r)}{D} v\,(C_1\chi(r) + C_2\varphi(r)), \\ C_2' &= \frac{\chi(r)}{D} v\,(C_1\chi(r) + C_2\varphi(r)), \end{aligned}\right\} \tag{21.14}$$

where to simplify the notation we dropped all the indices of $\chi_{nl}^{(0)}$ and $\varphi_{nl}^{(0)}$ and wrote

$$\left.\begin{aligned} v(r) &= k_{nl}^2 - (k_{nl}^{(0)})^2 - w, \\ D &= \varphi\chi' - \varphi'\chi. \end{aligned}\right\} \tag{21.15}$$

Equations (21.14) can be solved by perturbation theoretical methods. In the first approximation, we take in the right-hand side of these equations $C_1 = 1$ and $C_2 = 0$. Moreover, we should remember that the wave function must everywhere be bounded, so that we should have

$$C_2(0) = C_2(\infty) = 0, \tag{21.16}$$

since φ diverges at the origin as r^{-l} and at infinity as $e^{|k_{nl}^{(0)}|r}$. All this combined gives

$$\left.\begin{aligned} C_1(r) &= 1 - \frac{1}{D}\int_0^r v(\rho)\,\chi(\rho)\,\varphi(\rho)\,d\rho, \\ C_2(r) &= \frac{1}{D}\int_0^r v(\rho)\,\chi^2(\rho)\,d\rho. \end{aligned}\right\} \tag{21.17}$$

The first condition in (21.16) is clearly satisfied. From the second condition we find k_{nl}^2 in this approximation:

$$\Delta^{(1)}(k_{nl}^2) = (k_{nl}^{(1)})^2 - (k_{nl}^{(0)})^2 = \int_0^\infty w(\rho)\,\chi^2(\rho)\,d\rho. \tag{21.18}$$

The normalization $\int_0^\infty \chi^2(\rho)d\rho = 1$.

Expressions (21.12) and (21.17) give a closed expression for the perturbed wave function of a bound state to first order in w. Expression (21.18), defining the bound-state energy correction, adds nothing to the usual expression of the first approximation of the perturbation theory. The advantages of this method become apparent only in calculating the energy corrections in higher approximations. As an example, let us derive the energy correction in the second approximation. Inserting (21.17) in the right-hand side of (21.14), we can find $C_2(r)$ by elementary means. The condition $C_2(\infty) = 0$ directly gives for the energy shift

$$\Delta^{(2)}(k_{nl}^2) = \Delta^{(1)}(k_{nl}^2) + \frac{1}{2D}\int_0^\infty\int_0^\infty d\rho\, d\sigma\, [\Delta^{(1)}(k_{nl}^2) - w(\rho)]\, [\Delta^{(1)}(k_{nl}^2) - w(\sigma)] \times \\ \times \chi(\rho)\chi(\sigma)[\chi(\rho)\varphi(\sigma) + \varphi(\rho)\chi(\sigma)]. \tag{21.19}$$

This expression, like all the others obtained by this method, does not include the complete set of functions of the unperturbed equation, but only the two functions φ and χ. The introduction of the irregular solution is thus equivalent to the introduction of a complete set of everywhere regular functions χ_{nl}, χ_{kl}!

As the Wronskian D is independent of r, we can express φ in terms of χ:

$$\varphi(r) = -\chi(r) D \int_a^r \frac{d\rho}{\chi^2(\rho)}. \tag{21.20}$$

This means that the entire perturbation theory can actually be developed using only the regular unperturbed solution χ_{nl}.

§ 22. PERTURBATION THEORY: MOMENTUM REPRESENTATION

Let us consider the equations of the perturbation theory in the momentum representation. The momentum formulation of the perturbation theory is actually used in field theory, and certain difficulties and singularities encountered in this advanced treatment can be understood within the framework of nonrelativistic quantum mechanics.

We start with the ordinary Sch. Eq.

$$\left(-\frac{\hbar^2}{2m}\Delta + U - E\right)\psi_k(r) = 0.$$

The wave function $\psi_k(r)$ is replaced by its Fourier transform (or in other words, we change over to the momentum representation):

$$\left.\begin{aligned} \psi_k(r) &= \frac{1}{(2\pi)^{3/2}}\int e^{iqr}\varphi_k(q)\, dq, \\ \varphi_k(q) &= \frac{1}{(2\pi)^{3/2}}\int e^{-iqr}\psi_k(r)\, dr. \end{aligned}\right\} \tag{22.1}$$

The equation for $\varphi_k(q)$ (the Schroedinger equation in momentum representation) takes the form

$$(q^2 - k^2)\varphi_k(q) = -\int V_{qq'}\varphi_k(q')\, dq', \tag{22.2}$$

where

$$V_{qq'} = \frac{1}{(2\pi)^3}\int e^{-i(q-q')r}V(r)\,dr. \tag{22.3}$$

The equation of free motion ($V(r) = 0$) with a source in the right-hand side

$$(q^2 - k^2)\,\varphi_k(q) = Q(q) \tag{22.4}$$

has a particular solution

$$\varphi_k(q) = \frac{Q(q)}{q^2 - k^2 \mp i\gamma}, \quad \gamma \to +0, \tag{22.5}$$

whence we conclude that the function

$$g_k^{(\pm)}(q) = \frac{1}{q^2 - k^2 \mp i\gamma} \tag{22.6}$$

is Green's function of the Schroedinger equation in the momentum representation. Just as in the coordinate representation, the signs ± correspond to two independent Green's functions meeting different conditions at infinity (an incoming and outgoing wave).

In (22.5) changing over to the coordinate representation we get

$$\psi_k(r) = \frac{1}{(2\pi)^{3/2}}\int e^{iqr}\varphi_k(q)\,dq = \frac{1}{(2\pi)^{3/2}}\int e^{iqr}\,\frac{Q(q)}{q^2 - k^2 \mp i\gamma}\,dq. \tag{22.7}$$

The vector r is chosen as the polar axis, and $Q(q)$ is written in explicit form as a function of the Cartesian coordinates:

$$Q(q) = Q(q_x, q_y, q_z).$$

Taking $\xi = \frac{qr}{qr}$, we obtain

$$\psi_k(r) = \frac{1}{(2\pi)^{3/2}}\int_0^{2\pi} d\varphi \int_{-1}^{1} d\xi \int_0^{\infty} \frac{q^2}{q^2 - (k^2 \pm i\gamma)}\,e^{iqr}\times$$
$$\times\, Q\left(q\sqrt{1-\xi^2}\cos\varphi,\ q\sqrt{1-\xi^2}\sin\varphi,\ q\xi\right)dq.$$

Parts integration over ξ gives

$$\int_{-1}^{1} d\xi e^{iqr\xi}Q = \frac{1}{iqr}\left\{e^{iqr}Q(0,0,q) - e^{-iqr}Q(0,0,-q)\right\} - \frac{1}{iqr}\int_{-1}^{1} e^{iqr\xi}\frac{\partial Q}{\partial \xi}\,d\xi.$$

The last integral (as further integration by parts will show) is of the order of $\frac{1}{r^2}$ and can be dropped from the asymptotic expression. Thus (we write $Q(q)$ for $Q(0, 0, q)$)

$$\psi_k(r) \sim \frac{1}{(2\pi)^{3/2}}\frac{1}{ir}\int_0^{\infty} \frac{q\,dq}{q^2 - (k^2 \pm i\gamma)}\left[e^{iqr}Q(q) - e^{-iqr}Q(-q)\right] =$$
$$= \frac{1}{2ir}\frac{1}{(2\pi)^{3/2}}\int_{-\infty}^{\infty} \frac{q\,dq}{q^2 - (k^2 \pm i\gamma)}\left[e^{iqr}Q(q) - e^{-iqr}Q(-q)\right]. \tag{22.8}$$

For simplicity let $Q(q)$ as a function of the complex variable q have no singularities in the upper halfplane. * In this case integration of the first term in brackets can be carried out using a contour which is completed in the upper halfplane and of the second term using a contour completed in the lower halfplane. The integrand has poles at the points $q = \pm (k \pm i\gamma)$ and we find

$$\psi_k^{(+)}(r) \sim \frac{e^{ikr}}{r}\sqrt{\frac{\pi}{2}}\,Q(k),\quad Q(k) = Q(0, 0, k) = Q\left(k\frac{r}{r}\right), \tag{22.9}$$

if we use $g_k^{(+)}(q)$.

$g^{(+)}$ thus corresponds to outgoing waves.

It can also be readily shown that the Green's function

$$g_k^{(-)}(q) = \frac{1}{q^2 - (k^2 - i\gamma)} \tag{22.10}$$

generates an incoming wave:

$$\psi_k^{(-)}(r) = \frac{1}{(2\pi)^{3/2}}\int e^{iqr}\,\frac{Q(q)}{q^2 - k^2 + i\gamma}\,dq \sim \frac{e^{-ikr}}{r}\sqrt{\frac{\pi}{2}}\,Q\left(-k\frac{r}{r}\right). \tag{22.11}$$

We can now readily write the perturbation theoretical expression for equation (22.2). Note that the solution of the free equation clearly has the form $\varphi_k(q) = \delta(k - q)$. In the coordinate representation this solution gives a plane wave

$$\frac{1}{(2\pi)^{3/2}}\,e^{ikr}.$$

Considering the right-hand side of (22.2) as an inhomogeneity, we can write the general solution of this equation as a sum of the solution of the homogeneous and inhomogeneous equations:

$$\varphi_k(q) = \delta(k - q) - g_k^{(+)}(q)\int dq' V_{qq'}\varphi_k(q'). \tag{22.12}$$

We thus obtain an integral equation for the wave function. Iterating we obtain the perturbation theoretical series

$$\varphi_k(q) = \delta(k - q) - g_k^{(+)}(q)\,V_{qk} + \int g_k^{(+)}(q)\,V_{qq'}\,g_k^{(+)}(q')\,V_{q'k}\,dq'. \tag{22.13}$$

This series is very often encountered in field theory and in related branches of physics.

* These singularities at points $q = q_1 + iq_2\,(q_2 > 0)$ would have given rise to terms of the form $e^{i(q_1 r - q_2 r}$, which make no contribution to the asymptotic behavior of ψ_k.

§ 23. CONVERGENCE OF THE PERTURBATION THEORETICAL SERIES

The applicability of the perturbation theory constitutes a fairly delicate problem, * of which only one aspect is considered here. In calculations one generally makes use of the following test: if the first approximation of the perturbation theory is much less than the zeroth approximation, and the second is much less than the first, this is taken as a sign that the perturbation theoretical series converges and only the first terms need be retained. In general, however, this is not so. We will demonstrate this fallacy for the case of the Sch. Eq. in the momentum representation. (Compare with the solution of this problem in the coordinate representation /154, 155/.)

We will obtain an exact solution of the problem and then try to solve it using the perturbation theoretical series. Consider the particular case of a singular potential (see § 3)

$$V(r) = -V_0 \text{ for } r < a \text{ and } V(r) = 0 \text{ for } r > 0$$

with $V_0 \to \infty$ and $a \to 0$, so that $V_0 a^2 \to \text{const}$. At the first stage, however, we take V_0 and a to be constant. The matrix element $V_{qq'}$ of this potential entering equation (22.2) is

$$V_{qq'} = -\frac{V_0}{2\pi^2} \frac{1}{|q-q'|^3} \{\sin(a|q-q'|) - a|q-q'|\cos(a|q-q'|)\}. \tag{23.1}$$

For $|q-q'|a \ll 1$, series expansion gives

$$V_{qq'} = -\frac{V_0 a^3}{6\pi^2}; \tag{23.2}$$

for $|q-q'|a \gg 1$ the matrix element falls off rapidly while oscillating:

$$V_{qq'} \sim \frac{V_0 a}{2\pi^2 |q-q'|^2} \cos a|q-q'| < \frac{V_0 a^3}{6\pi^2}. \tag{23.3}$$

The principal contribution is clearly from the region $|q-q'| < \frac{1}{a}$. We will therefore first consider a potential with sharp cutoff:

$$V_{qq'} = \begin{cases} -C \text{ for } |q| \text{ and } |q'| < b, \\ 0 \text{ for } |q| \text{ or } |q'| > b, \end{cases} \tag{23.4}$$

where $C \to 0$, $b \to \infty$ for $a \to 0$.

* For example, the application of the perturbation theory to the hydrogen atom (the entire Coulomb potential is treated as a perturbation) gives in the second approximation a finite, but incorrect energy /148, 149/. In the presence of bound states the perturbation theoretical series may diverge starting at a certain energy. This difficulty is sometimes avoided by using alternative methods, e.g., Fredholm's method /150—152/ or the method of quasiparticles /153/. In the case of a highly singular repulsion potential, the perturbation theoretical series diverges, whereas the physical result is bounded. A development of this kind possibly arises in the so-called nonrenormalizable quantum field theories (see, e.g., /237/).

Equation (22.2) is written in the following form:

$$(q^2 - k^2)\,\varphi_k(q) = 4\pi C \int_0^b q'^2 \varphi_k(q')\,dq'. \tag{23.5}$$

If we are interested in the bound state of the particle (i.e., $k^2 = -|k^2| = -\varkappa^2$), we choose a solution in the form

$$\varphi_k(q) = \begin{cases} \frac{A}{q^2 - k^2} & \text{for } q \leqslant b, \\ 0 & \text{for } q > b \end{cases} \tag{23.6}$$

and insert it in the equation to obtain after elementary integration

$$0 = 1 - 4\pi C \int_0^b \frac{q'^2\,dq'}{q'^2 + \varkappa^2} = 1 - 4\pi C \left[b - \varkappa \tan^{-1}\frac{b}{\varkappa}\right] \xrightarrow[b\to\infty]{} 1 - 4\pi C\left[b - \frac{\pi}{2}\varkappa\right]. \tag{23.7}$$

Hence we find the binding energy (or more precisely, the corresponding wave vector)

$$\varkappa = \frac{4\pi C b - 1}{2\pi^2 C}. \tag{23.8}$$

We have so far regarded a, V_0, C, and b as finite. In the limit as $a \to 0$, $V_0 \to \infty$ we have from the preceding $C \to 0$, $b \to \infty$. If we wish to preserve constant bound-state energy on passing to a singular potential, b should go to infinity for $a \to 0$ as

$$\frac{1 + 2\pi^2 C\varkappa}{4\pi C}. \tag{23.9}$$

Using (23.6) we readily find the wave function in the coordinate representation:

$$\psi(r) = \frac{1}{(2\pi)^{3/2}} \int e^{iqr} \varphi_k(q)\,dq = A \frac{2^{1/2}}{\pi} \frac{e^{-\varkappa r}}{r}, \tag{23.6'}$$

and from the normalization condition we find the constant A, i.e., $A = \sqrt{2\varkappa/\pi}$.

The wave function (23.6') diverges at the origin, as is proper for a singular potential.

Now consider the problem of scattering. The wave function is sought in the form

$$\varphi_k(q) = \delta(k - q) + \frac{B}{q^2 - (k^2 + i\gamma)}, \tag{23.10}$$

where γ is an infinitesimal positive number. We will see in what follows that this form indeed corresponds to the scattering problem: on passing to the coordinate representation, the first term gives a plane wave and the second term gives a scattered outgoing wave. Inserting (23.10) in the starting equation and using (23.4) and the identity

$$\frac{1}{q^2 - (k^2 + i\gamma)} = \frac{1}{q^2} + \frac{k^2 + i\gamma}{q^2(q^2 - k^2 - i\gamma)}, \tag{23.11}$$

we reduce the equation to the form

$$0 = B - C\left\{1 + 4\pi B\int_0^b \frac{q^2\,dq}{q^2-(k^2+i\gamma)}\right\} \equiv B - C\left\{1 + 4\pi B\left(b + \frac{\pi i k}{2}\right)\right\}.$$

Using (23.8), we rewrite this as

$$B = \frac{i}{2\pi^2}\,\frac{1}{k - i\varkappa},$$

which solves our problem of finding the wave function.

Reverting to the coordinate representation, we get

$$\psi_k(r) = \frac{1}{(2\pi)^{3/2}}\left\{e^{ikr} + \frac{i}{k-i\varkappa}\,\frac{e^{ikr}}{r}\right\}. \tag{23.12}$$

The scattering cross section is

$$\sigma = \frac{4\pi}{\varkappa^2}\,\frac{\varkappa^2}{\varkappa^2 + k^2}. \tag{23.13}$$

Let us try to solve the same problem with a singular potential using the perturbation theory. At a first glance, this would appear to be very simple, as the matrix elements of the interaction $V_{qq'}$ go to zero for $q \to 0$.

The perturbation theoretical procedure calls for iteration of the starting equation (23.5). The unperturbed wave function (i.e., the solution of this equation without the right-hand side) is simply a plane wave:

$$\varphi_k^{(0)}(q) = \delta(k - q).$$

The first-approximation correction is (see previous section)

$$\varphi_k^{(1)}(q) = \frac{-V_{qk}}{q^2 - k^2 - i\gamma} = \begin{cases} \dfrac{C}{q^2 - k^2 - i\gamma} & \text{for } q < b, \\ 0 & \text{for } q > b. \end{cases}$$

Inserting this expression in the right-hand side of (23.5), we find

$$\varphi_k^{(2)}(q) = \frac{C}{q^2 - k^2 - i\gamma}\,4\pi C\left(b + \frac{i\pi k}{2}\right).$$

Reiterating, we find

$$\varphi_k^{(n)}(q) = \frac{C}{q^2 - k^2 - i\gamma}\left[4\pi C\left(b + \frac{i\pi k}{2}\right)\right]^{n-1}. \tag{23.14}$$

Finally, to obtain the exact wave function we should sum the entire infinite perturbation theoretical series, which in our case is easily accomplished, as the series reduces to a simple geometrical progression:

$$\begin{aligned} \varphi_k(q) &= \delta(k - q) + \sum_{n=1}^{\infty} \varphi_k^{(n)}(q) = \\ &= \delta(k - q) + \frac{C}{q^2 - k^2 - i\gamma}\,\frac{1}{1 - 4\pi C\left(b + \frac{i\pi k}{2}\right)} = \\ &= \delta(k - q) + \frac{i}{2\pi^2(k - i\varkappa)}\,\frac{1}{q^2 - k^2 - i\gamma}, \end{aligned} \tag{23.15}$$

and the result coincides with the previous exact expression.

We have seen in the preceding that each approximation of the perturbation theory vanishes in the limit as $C \to 0$, i.e., when the range of the potential goes to zero. However, the final result, which is a sum of an infinite series, is nevertheless different from zero, as it depends not on the range of the potential but only on the energy of the bound state. This is a clear proof of the fact that smallness of the first and higher terms of the perturbation theoretical series does not guarantee sufficiently fast convergence of the entire series. The reason is fairly simple: the applicability test of the perturbation theory is that the wave function increment $\Delta\varphi(q)$ be much less than the zeroth approximation function for all values of the argument.

For the case under discussion, the zeroth approximation function $\varphi_k^{(0)}(q)$ is zero for $k \neq q$. The corrections $\varphi_k^{(n)}(q)$, on the other hand, do not vanish virtually for all q, although in absolute value they go to zero. As the result, any finite number of approximations does not give a correct answer for the wave function.

We have assumed, as is the common practice, that for a sufficiently small perturbation λW and $\lambda \to 0$, the wave function ψ and the perturbed energy E can be expanded in powers of λ or, in other words, these functions are assumed to be analytic in λ.

This is however not always so. We will now give an example when the energy E is not an analytic function of λ. Let $\varphi_0, \ldots, \varphi_N$ and $E_0 = 0, \ldots, E_N$ be the eigenfunctions and the eigenvalues of the unperturbed Hamiltonian

$$H_0\varphi_0 = E_0\varphi_0, \quad H_0\varphi_n = E_n\varphi_n, \quad n = 1, \ldots, N,$$

where E_n are uniformly distributed over the interval $(-\Delta, \Delta)$. Further let the interaction Hamiltonian have nonzero matrix elements only between the states 0 and n, all elements having the same sign. Finally, to simplify the mathematics, let all the matrix elements be equal, $V_{0n} = V$.

The solution of the Sch. Eq.

$$(E - H_0)\psi = V\psi$$

is sought in the form

$$\psi = A\left(\varphi_0 + \sum_{n=1}^{N} c_n\varphi_n\right). \tag{23.16}$$

It is assumed that $c_n \ll 1$. For these coefficients we readily obtain the equations

$$E = V\sum_{n=1}^{N} c_n, \quad (E - E_n)c_n = V. \tag{23.17}$$

Solving the second equation for c_n and inserting the result in the first equation, we obtain

$$E = f(E) = V^2\sum_{n=1}^{N}\frac{1}{E - E_n}. \tag{23.18}$$

This is an exact equation for the energy E. We see from Figure 13 that the equation has $(N-1)$ roots over the interval $[-\Delta, \Delta]$, one root for $E > \Delta$ and one root for $E < -\Delta$.

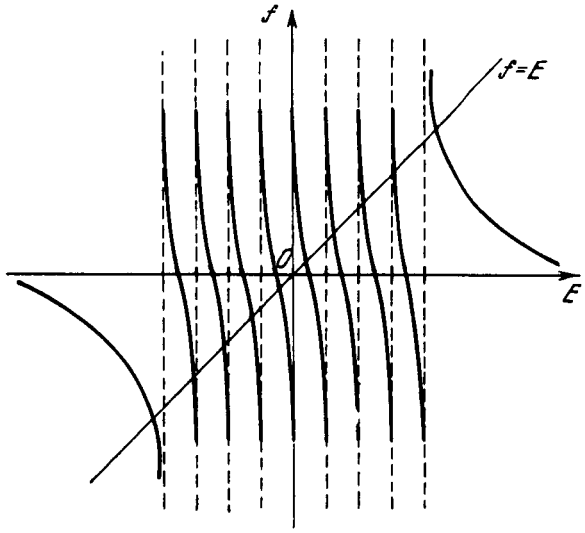

FIGURE 13.

Let us find the ground state energy in the limit as $N \to \infty$ (the root of the equation for $E < -\Delta$). In this case, the sum can be replaced by an integral, so that

$$\frac{E}{\Delta} = -\frac{NV^2}{2\Delta^2} \ln \frac{E-\Delta}{E+\Delta}. \tag{23.19}$$

We obtained a transcendental equation for E. Note that for the effective coupling to remain weak (it is this case that we consider) it is necessary that for $N \to \infty$, $V \to 0$ so that the prelogarithmic coefficient goes to a small number, i.e., $\frac{NV^2}{2\Delta^2} \to \alpha \ll 1$. In this case $E \approx -\Delta$ and we get

$$E + \Delta = -2\Delta e^{-\frac{1}{\alpha}}, \quad \alpha = \lim_{N\to\infty} \frac{NV^2}{2\Delta^2} \ll 1. \tag{23.20}$$

We obtained an expression for the ground state energy, which is a non-analytic function of the perturbation force V and therefore cannot be recovered from perturbation theory. Note that in our case the distance between levels in the interval $[-\Delta, \Delta]$ is of the order of $\frac{2\Delta}{N}$ and therefore approaches zero for $N \to \infty$, when the distance between the lowermost level and the next higher level is finite, being equal to $\Delta_1 = E + \Delta = -2\Delta e^{-\frac{1}{\alpha}}$. We obtained a so-called energy slit, plus a continuum in the interval

$[-\Delta, \Delta]$. Note that the probability A^2 of finding the state φ_0 in the ground state ψ_0 is finite in our case:

$$A^2 \approx \frac{2}{\alpha} e^{-\frac{1}{\alpha}}. \tag{23.21}$$

The above model probably appears to be highly artificial, without any relation to actual practical problems.

In this respect we should emphasize that it may be treated as a model (though very rough) of the superconducting state. Here the function φ_n corresponds to the states φ_k of a pair of electrons with oppositely directed momenta k and $-k$ and spins (Cooper pairs /156/), and 2Δ can be interpreted as the thickness of the Fermi surface (this is the region where the superconducting interaction takes place). The interaction between different states in this model is associated with transitions to an intermediate state φ_0 and is called effective attraction. This model qualitatively reproduces the characteristic features of the superconducting state: the formation of the slit for arbitrarily weak attraction and the nonanalytical dependence of slit width on the interaction force /157, 158/.

§ 24. DIAGRAM TECHNIQUE

The widespread use of the perturbation theoretical series in modern theoretical physics suggested the development of standardized computation procedures which had to be made as graphically meaningful as possible. This was accomplished with the advent of the diagram technique, invented by Feynman at the end of the 1940's /159/. This technique originally evolved from problems of quantum electrodynamics, but now it is almost in universal use.

The diagram technique is conveniently applicable to nonrelativistic quantum mechanics. We will now describe how this technique is developed.

Consider the Sch. Eq. with a perturbation $W(r)$:

$$(H_0 - E)\psi = \left(-\frac{\hbar^2}{2m}\Delta + U - E\right)\psi = -W\psi. \tag{24.1}$$

Complete systems of wave functions of the unperturbed operator $(H_0 - E)$ will be denoted by $\psi_k^{(\pm)}(r)$ and Green's function by $G_E^{(+)}(r, r')$. The solution is sought in the form

$$\psi(r) = \psi_{k_0}^{(+)}(r) + \varphi_{k_0}(r),$$

where the increment $\varphi_{k_0}(r)$ is regarded as small. For $\varphi_{k_0}(r)$ we obtain the equation

$$(H_0 - E)\varphi_{k_0} = -W(r)(\psi_{k_0}^{(+)} + \varphi_{k_0}). \tag{24.1'}$$

Iteration of this equation yields

$$\varphi_{k_0}(r) = \sum_{n=1}^{\infty} \varphi_{k_0}^{(n)}(r),$$
$$\varphi_{k_0}^{(n)}(r) = (-1)^n \int dr_1 \dots$$
$$\dots dr_n G_E^{(+)}(r, r_n) W(r_n) G_E^{(+)}(r_n, r_{n-1}) W(r_{n-1}) \dots$$
$$\dots W(r_2) G_E^{(+)}(r_2, r_1) W(r_1) \psi_{k_0}^{(+)}(r_1). \qquad (24.2)$$

We are generally concerned only with the asymptotic behavior for $r \to \infty$. In this case, using expression (18.3), we find

$$\varphi_{k_0}^{(n)}(r) \sim \frac{e^{ikr}}{r}(-1)^n \frac{2m}{\hbar^2} \int dr_1 \dots$$
$$\dots dr_n \psi_k^{(-)*}(r_n) W(r_n) G_E^{(+)}(r_n, r_{n-1}) \dots$$
$$\dots W(r_2) G_E^{(+)}(r_2, r_1) W(r_1) \psi_{k_0}^{(+)}(r_1) = \frac{e^{ikr}}{r} f^{(n)}(k, k_0),$$
$$\varphi_{k_0}(r) = \frac{e^{ikr}}{r} f(k, k_0); \quad f(k, k_0) = \sum_{n=1}^{\infty} f^{(n)}(k, k_0), \qquad (24.3)$$

where $k = k\frac{r}{r}$.

We see from these expressions that the amplitudes $f^{(n)}$ have an attractively simple structure: first comes in the rightmost position the unperturbed function $\psi_{k_0}^{(+)}$, which describes the primary particle wave propagating in the direction k_0. Then come alternating the functions W and $G^{(+)}$ and finally, in the leftmost position we have the function $(\psi_k^{(-)})^*$ which describes the scattered wave propagating in the direction k. Each amplitude $f^{(n)}(k, k_0)$ can be put in correspondence with a simple graph or diagram.

As an example, we will draw the diagrams corresponding to first few amplitudes (Figure 14). A one-to-one correspondence between diagrams and amplitudes is established as follows: the line from infinity to the point r_1 is made to correspond to the initial function $\psi_{k_0}^{(+)}(r_1)$, a cross at a point r_i corresponds to the function $(-W(r_i))$, a line joining two adjacent points r_i and r_{i+1} to the function $G_E^{(+)}(r_i, r_{i+1})$, and a line going to infinity from the last vertex to the wave function of the final state $\psi_k^{(-)*}(r_n)$. To calculate the amplitude $f^{(n)}$, we should assemble the product following the above prescription and then integrate over the coordinates of all the vertices. The integral is then multiplied by $\frac{2m}{\hbar^2}$ (see (24.3)). The amplitude $f^{(n)}$ is represented by a graph with n vertices.

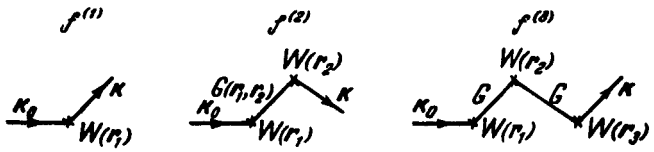

FIGURE 14.

Each diagram has a simple physical meaning. The line drawn from infinity corresponds to a particle moving from infinity (in the initial

direction k_0) in the unperturbed potential U. This particle is scattered at the point r_1 by the perturbation W, resumes its motion in the field U, reaches the point r_2, where it is again scattered by the perturbation W, eventually reaching the point r_3, and so on. The particle scattered for the last time by W at the point r_n escapes to infinity (moving in the direction of the vector k). Between two successive scattering events the motion of the particle is described by Green's function $G^{(+)}(r_i, r_{i+1})$. This function is therefore often called the propagation function or propagator.

In this simple case the graphs clearly contribute toward better intuitive understanding of the problem, but hardly simplify the mathematics: the structure of the original perturbation theoretical series is as simple as they come.

In more complicated problems, however, the graphs are quite helpful in mathematical manipulations. Consider, for example, the case of several perturbations

$$W = W_1 + W_2.$$

If $(-W_1)$ corresponds to a cross and $(-W_2)$ to a circle, then following the above prescription we have two amplitudes in the first approximation (Figure 15) and four amplitudes in the second approximation (Figure 16). As the order of the perturbation theoretical approximation increases, the number of terms making up the amplitude grows catastrophically. The use of graphs greatly simplifies the problem of drawing up the complete perturbation theoretical series and safeguards against omission of individual terms.

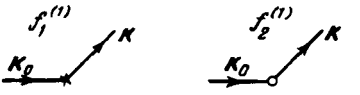

FIGURE 15.

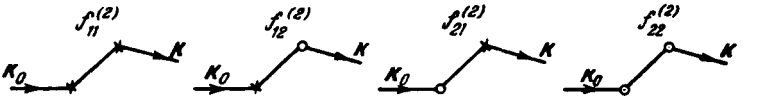

FIGURE 16.

In field theory we generally work in the momentum representations and all the interactions are incorporated in the perturbation W. Expression (24.3) can be rewritten in an alternative form remembering that in this case

$$\psi_k^{(+)} = \psi_k^{(-)} = \frac{1}{(2\pi)^{3/2}} e^{ikr},$$

$$G_E^{(+)}(r, r') = -\int dp \frac{\psi_p^{(+)}(r)\,(\psi_p^{(+)})^*(r')}{E - E_p + i\gamma}.$$

Inserting these functions in (24.3), we obtain after elementary manipulations

$$f^{(n)}(\boldsymbol{k}, \boldsymbol{k}_0) = \frac{2m}{\hbar^2}\int dq_1 \ldots dq_n V_{kq_n} \frac{1}{E - E_{q_n} + i\gamma} \times \\ \times V_{q_n q_{n-1}} \frac{1}{E - E_{q_{n-1}} + i\gamma} \ldots V_{q_1 q_1} \frac{1}{E - E_{q_1} + i\gamma} V_{q_1 k_0}. \tag{24.3'}$$

Here the propagators are $\frac{1}{E - E_{q_i} + i\gamma}$, and the vertices of the graphs correspond to the Fourier components of the potential.

§ 25. TIME-DEPENDENT GREEN'S FUNCTION

Consider the inhomogeneous time-dependent Sch. Eq.

$$\left(i\hbar\frac{\partial}{\partial t} - H\right)\varphi(\boldsymbol{r}, t) = Q(\boldsymbol{r}, t). \tag{25.1}$$

A particular solution of this equation can be written in the form

$$\varphi(\boldsymbol{r}, t) = \int d\boldsymbol{r}'\, dt' G(\boldsymbol{r}, t; \boldsymbol{r}', t') Q(\boldsymbol{r}', t'). \tag{25.2}$$

The time-dependent Green's function here is

$$G = -\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dE G_E(\boldsymbol{r}, \boldsymbol{r}') e^{-\frac{iE(t-t')}{\hbar}}. \tag{25.3}$$

Indeed, seeing that

$$HG_E = EG_E + \delta(\boldsymbol{r} - \boldsymbol{r}'),$$

we readily find

$$\left(i\hbar\frac{\partial}{\partial t} - H\right)G(\boldsymbol{r}, t; \boldsymbol{r}', t') = \frac{1}{2\pi\hbar}\int dE\, \delta(\boldsymbol{r} - \boldsymbol{r}') e^{-\frac{iE(t-t')}{\hbar}} = \delta(\boldsymbol{r} - \boldsymbol{r}')\delta(t - t'). \tag{25.4}$$

Expression (25.3) is not single-valued, as we may use either $G_E^{(+)}$ or $G_E^{(-)}$.

We will see presently that the first alternative (i.e., $G_E^{(+)}$) is of the greatest practical importance. It describes the natural evolution of events from past to future. We will therefore consider this case only.

Using the explicit expression for $G^{(+)}$ we write

$$G(\boldsymbol{r}, t; \boldsymbol{r}', t') = \frac{1}{2\pi\hbar}\int dE e^{-\frac{i}{\hbar}E(t-t')}\int d\boldsymbol{p}\, \frac{\psi_{\boldsymbol{p}}^{(+)}(\boldsymbol{r})\,\psi_{\boldsymbol{p}}^{(+)*}(\boldsymbol{r}')}{E - \left(\frac{\hbar^2 p^2}{2m} - i\gamma\right)}.$$

Integrating over E and remembering that $\gamma > 0$, we obtain

$$G(\boldsymbol{r}, t; \boldsymbol{r}', t') = \begin{cases} -\frac{i}{\hbar}\int d\boldsymbol{p}\, \psi_{\boldsymbol{p}}^{(+)}(\boldsymbol{r})\,\psi_{\boldsymbol{p}}^{(+)*}(\boldsymbol{r}')\, e^{-\frac{i}{\hbar}\frac{\hbar^2 p^2}{2m}(t-t')} & \text{for } t > t', \\ 0 & \text{for } t < t', \end{cases} \tag{25.5}$$

i.e., the function does not vanish only for $t > t'$.

The simplest Green's function is clearly that corresponding to the free Sch. Eq. Using (18.15) and (25.3)—(25.5), it can be written in any of the alternative forms

$$G_0^{(+)}(\mathbf{r}, t; \mathbf{r}', t') = -\frac{i}{\hbar}\left(\frac{m}{2\pi\hbar i (t-t')}\right)^{3/2} e^{i\frac{m(\mathbf{r}-\mathbf{r}')^2}{2\hbar(t-t')}} =$$

$$= -\frac{m}{4\pi^2\hbar^2}\int_{-\infty}^{\infty} dE \frac{e^{ik|\mathbf{r}-\mathbf{r}'| - \frac{iE}{\hbar}(t-t')}}{|\mathbf{r}-\mathbf{r}'|}. \qquad (25.6)$$

The solution of the free equation with a source $Q(\mathbf{r}, t)$ is given by

$$\varphi(\mathbf{r}, t) = -\frac{m}{4\pi^2\hbar^2}\int dE\, d\mathbf{r}'\, dt' Q(\mathbf{r}', t') \frac{e^{ik|\mathbf{r}-\mathbf{r}'| - i\frac{E(t-t')}{\hbar}}}{|\mathbf{r}-\mathbf{r}'|}. \qquad (25.7)$$

The meaning of this expression is crystal-clear: the wave function at a point $\mathbf{r}$ at time t is a superposition of waves converging at that point

$$\frac{e^{ik|\mathbf{r}-\mathbf{r}'| - i\frac{E}{\hbar}(t-t')}}{|\mathbf{r}-\mathbf{r}'|},$$

which left the point $\mathbf{r}'$ at time t'. The amplitude of these waves is determined by the source density $Q(\mathbf{r}', t')$. In the simplest case of a point source at the origin, which emits the wave at a time $t' = 0$ ($Q = \delta(\mathbf{r}')\,\delta(t')$), we have

$$\varphi(\mathbf{r}, t) = -\frac{i}{\hbar}\left(\frac{m}{2\pi i\hbar t}\right)^{3/2} e^{i\left(kr - \frac{Et}{\hbar}\right)}, \qquad (25.8)$$

where

$$k = \frac{m}{\hbar}\frac{r}{t}, \quad E = \frac{\hbar^2 k^2}{2m}.$$

Emission of particles with fixed energy ε corresponds to exponential dependence of source density on time:

$$Q(\mathbf{r}, t) = \tilde{Q}(\mathbf{r})\, e^{\frac{-i\varepsilon t}{\hbar}}. \qquad (25.9)$$

Indeed, in this case integration over t' and E in (25.7) is immediately carried out and we obtain

$$\varphi(\mathbf{r}, t) = -\frac{2m}{\hbar^2}\int d\mathbf{r}' \frac{1}{4\pi} \frac{e^{i\varkappa|\mathbf{r}-\mathbf{r}'| - \frac{i\varepsilon t}{\hbar}}}{|\mathbf{r}-\mathbf{r}'|} Q(\mathbf{r}'), \qquad (25.10)$$

where $\varkappa = \sqrt{\frac{2m\varepsilon}{\hbar^2}}$. If $\tilde{Q}$ does not vanish only in a small neighborhood around the point $\mathbf{r}'$, for large $\mathbf{r}$ we have the natural result

$$\varphi(\mathbf{r}, t) \underset{r\to\infty}{\sim} -\frac{2m}{\hbar^2}\frac{1}{4\pi}\frac{e^{i\varkappa r - \frac{i\varepsilon t}{\hbar}}}{r}\int d\mathbf{r}' e^{i\varkappa\frac{\mathbf{r}}{r}\mathbf{r}'}\tilde{Q}(\mathbf{r}'). \qquad (25.11)$$

This is clearly an outgoing wave of particles of energy ε. Its amplitude is the Fourier component of the source function.

Another Green's function whose explicit form is known is that of the harmonic oscillator $\left(U = \frac{m\omega^2 r^2}{2}\right)$

$$G(\mathbf{r}, t; \mathbf{r}', t') = -\frac{i}{\hbar}\left(\frac{m\omega}{2\pi i\hbar \sin\omega(t-t')}\right)^{3/2} e^{\frac{iS(\mathbf{r}, t; \mathbf{r}', t')}{\hbar}}, \tag{25.12}$$

where

$$S(\mathbf{r}, t; \mathbf{r}', t') = \frac{m\omega}{2\sin\omega(t-t')}[\cos\omega(t-t')(r^2 + r'^2) - 2\mathbf{r}\mathbf{r}']. \tag{25.13}$$

Note that $S(\mathbf{r}, t; \mathbf{r}', t')$ (like the exponent in (25.6)) is the classical action, i.e.,

$$S(\mathbf{r}, t; \mathbf{r}', t') = \int_{t'}^{t} L(\tau)\, d\tau,$$

where $L = T - U$ is the system Lagrangian, and the integral is taken over a classical trajectory of the particle. This is not an accidental result: it is closely related to the quasiclassical nature of motion in a potential $U(r)$ which is only a linear and quadratic function of position /160/. The potential U may be an arbitrary function of time in this case, $U = U(\mathbf{r}, t)$.

Chapter 5

QUASISTATIONARY STATES

§ 26. INTRODUCTION. GAMOW'S THEORY

In this chapter we meet with a new kind of effects: decay of radioactive nuclei or unstable particles and resonance scattering of particles. A great many events are associated with unstable states. Maximum attention is currently being devoted to investigation of resonance states of strongly interacting particles, briefly called resonances, which have been discovered in multitudes in recent years.

Strictly speaking, perfectly stable states are encountered very seldom. For example, of all the known "elementary" particles the only stable ones are the proton, the electron, the γ quantum, and the neutrino. Most of the nuclear states are unstable.

Excited states of atoms and nuclei constitute a special type of unstable states. In nonrelativistic quantum mechanics these states are generally treated as ordinary bound states. The interaction of the electrons with the radiation field is thus ignored, although it is responsible for transitions from upper to lower states with emission of γ quanta. In more precise treatment this interaction must be taken into consideration. It is significant that the same interaction (electromagnetic) produces two entirely different effects: it binds the electron to the nucleus and makes it jump from one state to another. Therefore, strictly speaking, we cannot simply turn off the interaction responsible for electronic transitions leaving on the interaction responsible for the existence of bound states. If this is done, the only stable level is found to be the ground state of the atom (the nucleus), with a continuum of states immediately adjoining it (the discrete spectrum is eliminated). The continuum states correspond to the scattering of a γ quantum by a ground-state nucleus. These delicate questions, however, are not discussed in what follows.

Instability effects can be described using the complete system of stationary states. However, this description involves a number of qualitative singularities. For example, when a particle is scattered by a potential well which is separated from the exterior region by a potential barrier, the particle wave function in the interior region (e.g., $\psi_E(0)$) markedly increases for certain $E = E_n$. In these cases the wave function $\psi_E(r)$ continued to the complex E plane is generally discovered to have a pole near E_n for $E = E_{0n}$. The corresponding solution of the Sch. Eq. gives rise to so-called quasistationary states, or states of complex energy.

The remarkable feature is that for quasistationary states we can define a norm and develop a perturbation theory analogous to that for stationary

states. Note, however, that at this time the theory of quasistationary states is still in a relatively embryonic stage, and manipulation of quasistationary states therefore requires extreme caution.

Fortunately, many other problems of the theory of quasistationary states can be elucidated with the aid of exactly solvable models. These problems include, e.g., the analytical properties of the wave function of a quasistationary state, the determination of the mean lifetime of an unstable particle from the scattering of its decay products by one another, the exponential character of decay of unstable particles, creation of unstable particles, asymptotic behavior of the wave function of a decaying particle for $r \to \infty$ and $t \to \infty$.

At the end of the chapter we will briefly consider other types of long-lived states (e.g., those corresponding to a virtual level).* Some aspects of the theory of unstable particles which can transform into one another (e.g., the problem of the electric dipole moment of an unstable particle) are treated in Chapter 8.

The first and the most important application of the concept of quasistationary states was the theory of alpha decay of heavy nuclei developed in 1928 by G. Gamow /161/ and independently, though somewhat later, by Gurney and Condon /162/.

This theory is still being used in the calculation of decay probabilities of radioactive nuclei; the probability of decay with the emission of one proton or two protons /163/ is also estimated using this theory. In historical retrospect, however, the significance of Gamow's theory is in that it constitutes the first successful application of quantum mechanics to the atomic nucleus.

We will briefly go over some well known starting facts: in a decay of a given nucleus, the α particles have a definite energy; thus, for example, in the decay $U_{92}^{238} \to Th_{90}^{234} + \alpha$ (the isotope Th_{90}^{234} is designated for historical reasons as UX_1), the energy of the α particle is 4.7 MeV. There is obvious electrostatic repulsion between the α particle and the daughter nucleus Th_{90}^{234}: the interaction potential is given by

$$U = \frac{Z_1 Z_2 e^2}{r} = \frac{2 \cdot 90 e^2}{r} = \frac{260}{r} \text{ MeV/fermi},$$

i.e., the potential is 4.7 MeV at a distance of 55 fermi. The range of nuclear forces is only of the order of the nuclear radius, i.e.,

$$1.2\, A^{1/3} \text{ fermi} = 1.2\, (234)^{1/3} \text{ fermi} = 7.4 \text{ fermi},$$

where the electric potential is approximately 35 MeV.

All that we know about the potential is summarized in Figure 17. The vertical axis gives the energy of the $Th_{90}^{234} + \alpha$ system; the distance between the α particle and the nucleus is laid off the horizontal axis. To the right of R, we are dealing with pure electrostatic potential; to the left of R the (negative) nuclear interaction is added. The state of the mother nucleus U_{92}^{238} corresponds to the energy E_1 marked by the dashed horizontal line, $E_1 = 4.7$ MeV. The resultant potential left of R should clearly be less than E_1. Between R and R_1 there is a region where $U > E_1$, i.e., a region where in classical theory the particle may not occur.

* Some qualitative features of nonstationary states in a periodic field (the so-called states with definite quasienergy) are discussed in /238–241, 17/.

Had the potential remained constant to the right of R (as shown by the dash-dotted line in Figure 17) instead of falling off to zero, the energy level E_1' would have been an ordinary stationary state. In this approximation we would have missed the main point, namely the decay; however, since the decay is an infrequent event (the decay time is $4.5 \cdot 10^9$ years!) the difference between E_1' and E_1 is negligible.

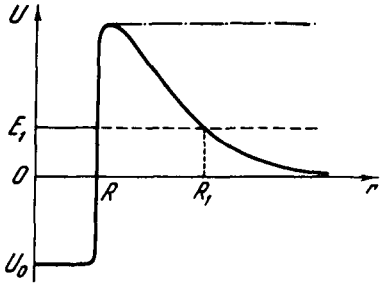

FIGURE 17.

To find the decay probability in the first approximation, we construct the wave function between R and R_1 in the quasiclassical approximation. In this approximation

$$r\psi = e^{\frac{i}{\hbar}\int p\,dx},$$

$$p = \sqrt{2m(E_1 - U)}$$

(p is the classical momentum corresponding to the total energy $E = \frac{p^2}{2m} + U$).

Under the barrier p is imaginary and the exponent in the expression for ψ is thus real. We thus have two independent solutions under the barrier, one increasing and the other decreasing (see § 2). The probability W of transmission through the barrier is proportional to the ratio $|\psi(R_1)|^2/|\psi(R)|^2$, which clearly should be computed for the decreasing solution, when it is minimum:*

$$W = e^{-\frac{2}{\hbar}\int_R^{R_1} \sqrt{2m(U-E_1)}\,dr}, \tag{26.1}$$

$$W = e^{-\frac{\pi Z_1 Z_2 e^2}{\hbar}\sqrt{\frac{2m}{E_1}}\left(1 - \frac{1}{\pi}(2\varphi_1 + \sin 2\varphi_1)\right)}, \tag{26.1'}$$

$$\varphi_1 = \sin^{-1}\sqrt{\frac{R}{R_1}}.$$

R_1 is determined as the point where $U - E_1 = 0$. Note that if the Coulomb potential $U(r)$ is extended to $R = 0$ and R is correspondingly replaced by zero as the lower limit of integration, the integral will converge to the simple result

$$W = e^{-\frac{\pi Z_1 Z_2 e^2}{\hbar}\sqrt{\frac{2m}{E_1}}} = e^{-\frac{2\pi Z_1 Z_2 e^2}{\hbar v_1}}; \tag{26.2}$$

* A derivation of (26.1) from the uncertainty relation can be found in /164/. The transmission of a wave packet through a potential barrier is treated in /165, 166/.

W — the transmission coefficient — is a nondimensional number. To find the decay probability w (the reciprocal of the decay time), the transmission probability should be multiplied by the number n of α particles impinging in unit time on the left wall of the barrier:

$$w = nW.$$

Here

$$n \sim \frac{R}{v} \sim \frac{R}{\sqrt{\frac{2(E_1 - U_0)}{m}}}.$$

This elementary expression* logically explains the fundamental property of α decay, namely the vanishingly low decay probability in case of a high barrier (for uranium $W \sim 10^{-37}$) and extreme sensitivity of the decay probability on E_1, the energy of the α particle.

It is clear that even if all the physical prerequisites of the theory are satisfied and we may actually discuss an individual α particle inside the nucleus, the pre-exponential factor is evaluated only approximately. Exact calculation of this factor is a complicated problem which requires knowledge of the behavior of the wave function ψ near the left turning point and it therefore essentially depends on the topography of the potential function inside the well.

According to the general theory, the situation depicted in Figure 17 is characterized by a continuum of real energies and nothing else. In principle, in addition to the continuum with $E > 0$, discrete levels with $E < 0$ are also possible, but clearly if $U_0 > 0$ there are none.

What is the meaning of the energy E_1? How are we to dissociate from the continuum one certain value of energy? A hint is supplied by the physical interpretation of the phenomenon. The wave function of a particle in the nucleus $(0 < r < R)$ falls off with time. Right of R_1, behind the barrier, there is a current of particles moving in the radial direction toward $r \to \infty$.

Remember that the stationary states from a continuum of real energies describe scattering of particles; the wave function far from the center is a superposition of the two wave functions $\frac{e^{-ip_0 r/\hbar}}{r}$ and $\frac{e^{ip_0 r/\hbar}}{r}$, i.e., a superposition of the incident wave and the outgoing wave; the amplitudes of these waves are identically equal in magnitude: the incident flux is equal to the reflected flux, i.e., particles are neither created nor destroyed.

For the description of α decay we demand that far from the force center there be only the outgoing wave. This does not contradict the particle number conservation, because $\int |\psi|^2 dr$ inside the nucleus decreases with time. The macroscopic equation of decay is

$$\frac{dN}{dt} = -wN; \quad N = N_0 e^{-wt},$$

* More detailed formulas and derivations will be found in /167/.

where N is the number of radioactive nuclei, i.e., the number of particles inside a sphere $r = R$. In the given ensemble, $N \sim \int |\psi|^2 dr$. We should thus seek a solution of the form

$$\psi = \psi(r)\, e^{-\frac{iE_1 t}{\hbar} - \frac{wt}{2}} = \psi(r)\, e^{-\frac{i}{\hbar}\left(E_1 - i\frac{\Gamma}{2}\right)} = \psi(r)\, e^{-\frac{i\widetilde{E}t}{\hbar}},$$

where $\widetilde{E} = E_1 - i\frac{\Gamma}{2}$ is a complex number; its imaginary part $\Gamma/2$ is related to the decay probability, $\Gamma = \hbar w$. * We can thus separate the variables in the nonstationary problem; $\psi(r, t)$ is sought as a product of $\psi(r)$ and an exponential function of t, just as in the stationary case.

The analogy is even more far-reaching: in time-independent problems discrete levels formed for $E < 0$, when for large r the linearly independent solutions had the form $e^{+|k|r}/r$ and $e^{-|k|r}/r$; the solution could be given the form $e^{-|k|r}/r$ for $r \to \infty$ only for certain discrete values of E.

Similarly, in time-dependent problems, we have two linearly independent solutions e^{ikr}/r and e^{-ikr}/r for large r, and the sought solution will have the desired form e^{ikr}/r for $r \to \infty$ only if we select a discrete complex value $\widetilde{E} = E_1 - i\Gamma/2$. Thus, the Sch. Eq.

$$i\hbar\frac{\partial\psi}{\partial t} = \left[-\frac{\hbar^2}{2m}\Delta + U(r)\right]\psi,$$

which is a partial differential equation, is reduced by the substitution $\psi = \psi(r)\, e^{\frac{-i\widetilde{E}t}{\hbar}}$ to an ordinary differential equation

$$\left[\widetilde{E} + \frac{\hbar^2}{2m}\frac{1}{r}\frac{d^2}{dr^2}r - U(r)\right]\psi(r) = 0, \tag{26.3}$$

and the boundary condition

$$\lim_{r\to\infty}\frac{d\ln r\psi}{dr} = \frac{i\sqrt{2m\widetilde{E}}}{\hbar} \tag{26.4}$$

takes care of the discrete complex values of E.

This is the way to solve the physical problem and to find the energy of particles inside the "radioactive" barrier $E_1 = \mathrm{Re}(\widetilde{E})$ and the lifetime of this state $\Gamma = -2\,\mathrm{Im}\,\widetilde{E}$ (the relation of Γ to the decay probability w was given above).

This procedure gives rise to numerous doubts as regards mathematical rigor and foundation; the most remarkable point, however, is that nobody questions the validity of the final result, i.e., the numerical values of E_1 and w; "only" the method of derivation is criticized. The main criticism is associated with the form of $\psi(r)$. Since $\widetilde{E}$ is a complex number, k is also complex. Asymptotically $\psi(r) \sim e^{ikr}/r$. It is readily verified that if the imaginary part of $\widetilde{E}$ is negative, we have

$$\left.\begin{aligned} k &= \frac{\sqrt{2mE_1}}{\hbar} - i\,\frac{\Gamma}{4\hbar}\sqrt{\frac{2m}{E_1}}, \\ \psi(r) &\sim e^{\frac{i\sqrt{2mE_1}}{\hbar}r}\,\frac{e^{\frac{\Gamma}{4\hbar}\sqrt{\frac{2m}{E_1}}r}}{r} \end{aligned}\right\} \tag{26.5}$$

* The method of complex eigenvalues was originated by J.J. Thomson /168/, who applied it to the problem of electromagnetic oscillations of charge on an ideally conducting sphere.

(we expanded $\sqrt{\widetilde{E}}$ taking $\Gamma \ll E_1$).

Thus the function $\psi(r)$ for $r \to \infty$ grows exponentially (though slowly, since Γ is small).* Such a function obviously cannot be normalized since $\int |\psi|^2 dr$ diverges. In the next sections we will show how the solution of a time-dependent partial differential equation $\psi(r, t)$ approaches the solution with separated variable $\psi(r) e^{-i\widetilde{E}t/\hbar}$. The normalized function $\psi(r, t)$ in a bounded region of space always approaches the non-normalizable $\psi(r) e^{-i\widetilde{E}t/\hbar}$.

In § 31 we will show that even for the non-normalizable $\psi(r)$ there is an expression that can be used as a norm in the perturbation theory and in determining the amplitude of $\psi(r)$ for an arbitrary initial state.

Here we will confine ourselves to a physical interpretation of the growth of $\psi(r)$ for $r \to \infty$. At any time t_0 we find at a given distance from the center those particles which were emitted, i.e., tunneled through the barrier, at a previous time $t = t_0 - r/v$, where v is the velocity of the particles. However, on account of the exponential time dependence, the amplitude ψ at the center at the earlier time was greater than it is at t_0. Indeed the factor $\left(\frac{\Gamma}{4\hbar}\sqrt{\frac{2m}{E_1}}\, r\right)$ can be written using the relation of Γ to w in the form $\exp\left(\frac{w}{2}\frac{r}{v}\right) = \exp\left(\frac{w}{2}(t_0 - t)\right)$. Hence it follows that $\psi(r, t_0) = \psi(0, t_0 - r/v)$.**

In conclusion note that all the theorems on the expansion of an arbitrary function in a complete system of eigenfunctions apply to the $\psi_E(r)$ for real E. Our $\psi_{\widetilde{E}}(r)$ is thus not included in the complete system of eigenfunctions, which is quite understandable in view of the nasty behavior of $\psi_{\widetilde{E}}(r)$ for $r \to \infty$.

The continuum eigenfunctions with real E close to $E_1 = \mathrm{Re}\,\widetilde{E}$ have a special form; we will see in the following that the complex energy $\widetilde{E}$ corresponds to a pole in the complex energy plane. On the other hand, for this very reason the determination of $\psi_{\widetilde{E}}(r)$ in a real problem with arbitrary $\psi(r, t = 0)$ requires application of a special technique, which differs from ordinary expansion in functions of a complete orthonormal system.

After this introduction we can proceed with a more detailed discussion of the entire gamut of problems associated with the existence of comparatively long-lived quasistationary states.

§ 27. WAVE FUNCTIONS

We have already mentioned that quasistationary states are identified with the poles of the scattering phase $S(k) = e^{2i\delta(k)}$ in the lower k halfplane. This approach enables us to obtain various general results with regard to the form and the energy dependence of the wave function for energies E close to the pole, to find the scattering cross section, etc.†

Consider the pole of $S(k) = e^{2i\delta(k)}$ at the point

$$k_0 = k_1 - ik_2$$

* It is on these grounds that Lamb /169/ objected to Thomson's method.

** Similar arguments were already brandished by Love /170/ in connection with Thomson's method.

† More detailed investigation of the analytical properties of wave functions will be found in /95, 171/.

in the complex plane. At this point, the wave function $\chi_k(r)$ defined by its asymptotic expansion (for simplicity we take $l = 0$ and consider uncharged particles)

$$\chi_k(r) \sim \sqrt{\frac{2}{\pi}} \sin(kr + \delta(k)) \tag{27.1}$$

identically goes to infinity for all r.

Let us establish the form of $S(k)$ near the pole. We recall that $S(k)$ should satisfy the symmetry conditions (13.5)—(13.6): it should have poles at the points k_0 and $-k_0^*$ and zeros at the points k_0^* and $-k_0$; on the real axis, $|S(k)| = 1$. The most general expression satisfying these condition is

$$S(k) = e^{2i\varphi(k)} \frac{(k - k_0^*)(k + k_0)}{(k - k_0)(k + k_0^*)}, \tag{27.2}$$

where $\varphi(k)$ is any function of k, which is real for real k and satisfies the symmetry properties (13.5), (13.6). As a rule $\varphi(k)$ is a sufficiently smooth function, so that near the pole it may be treated as constant (it is sometimes called the potential phase).

In scattering problems the energy and the wave vector of the particles are always real. The expression for the scattering phase is obtained from the general relation (27.2) where k should be regarded as a real positive number. For the scattering phase for $k_2 \ll k_1$, $k \sim k_1$ we get

$$\delta = \varphi - \tan^{-1} \frac{k_2}{k - k_1}. \tag{27.2'}$$

The wave vectors are generally replaced by energies:

$$\frac{\hbar^2}{2m}(k_1 - ik_2)^2 = \frac{\hbar^2}{2m}[(k_1^2 - k_2^2) - 2ik_1k_2] \equiv E_0 - \frac{i\Gamma}{2}. \tag{27.3}$$

Here E_0 is called the resonance energy, and Γ is the level width (the resonance width). Since in the k plane the poles lie in the lower halfplane, in the energy plane they lie on the second (the so-called unphysical) sheet of the Riemann surface; for $\Gamma \ll E_0$ and $E \sim E_0$ we can readily derive expressions analogous to (27.2) and (27.2'):

$$S(E) = e^{2i\varphi} \frac{E - E_0 - \frac{i\Gamma}{2}}{E - E_0 + \frac{i\Gamma}{2}}, \quad \delta = \varphi - \tan^{-1} \frac{\Gamma/2}{E - E_0}. \tag{27.4}$$

Using these expressions, we obtain for the scattering cross section

$$\sigma = \frac{\pi}{k^2}|S - 1|^2 = \frac{\pi}{k^2}\left\{\frac{\Gamma^2}{(E - E_0)^2 + \frac{\Gamma^2}{4}} - 4\mathrm{Re}\left[e^{i\varphi}\sin\varphi \frac{\Gamma}{E - E_0 + \frac{i\Gamma}{2}}\right] + 4\sin^2\varphi\right\}.$$

The first term here describes resonance scattering by the quasistationary state /172/, the last term corresponds to what is known as potential scattering, and the second term to interference of the two other terms.

Let the potential $V(r)$ have a finite range R. $\chi_k^{(0)}$ is the regular solution of the Sch. Eq. inside the potential range. We normalize this solution by

$$\int_0^R |\chi_k^{(0)}(r)|^2 dr = 1. \tag{27.5}$$

The total wave function is thus

$$\chi_k(r) = \begin{cases} A(k)\,\chi_k^{(0)}(r) & \text{for } r \leqslant R, \\ \sqrt{\frac{2}{\pi}}\sin(kr + \delta_0) & \text{for } r > R. \end{cases} \tag{27.6}$$

At the point $k = k_0$ this function should identically go to infinity. For $r > R$ this ensures an infinite $S(k)$ and thus an infinite scattering phase $\delta(k)$. In the interior region $\chi_k^{(0)}$ is bounded by assumption and the wave function may identically go to infinity only if the coefficient A in (27.6) is infinite.

The coefficient A is calculated without much difficulty. To this end we use the previously obtained expression (15.18). Inserting the scattering phase from (27.2) or (27.4) and retaining only the dominant term, we find

$$\int_0^R \chi_k^2 dr = \frac{\hbar}{\pi}\sqrt{\frac{2E_0}{m}}\frac{\Gamma/2}{(E-E_0)^2+\Gamma^2/4} \equiv A^2(k). \tag{27.7}$$

The average value of the wave function is clearly

$$\overline{\chi}_k \approx \frac{1}{R^{3/2}}A(k);\quad (\overline{\chi_k^2})_{\max} = \frac{1}{R}\frac{2\hbar v_0}{\pi\Gamma};\quad v_0 = \sqrt{\frac{2E_0}{m}}. \tag{27.7'}$$

Outside the barrier $\chi^2 \sim 1$, which is much less than the maximum particle density inside the barrier if Γ is sufficiently small. Physically this implies that particles accumulate in the region $r < R$: a particle entering this region remains there for some time before being allowed to escape outside. The particle lifetime inside the barrier is greater than the time of flight through this region $\tau = \frac{R}{v_0}$ by the same factor as the particle density inside is greater than the particle density outside. Hence we see that the mean lifetime τ_0 of a quasistationary state for $E \sim E_0$ is equal in its order of magnitude (more exact formulas will be given below) to

$$\tau_0 \sim \tau\frac{(\overline{\chi^2})_{\max}}{1} \sim \frac{R}{v_0}\frac{1}{R}\frac{\hbar v_0}{\Gamma} \sim \frac{\hbar}{\Gamma}. \tag{27.8}$$

This time may be very large, which explains the origin of the term "quasi-stationary state". We should again emphasize that expressions (27.7) and (27.8) apply to scattering problems; the energy E and the wave vector k are therefore both real.

Qualitative analysis of various particular cases shows that the strong dependence of the wave function on energy near certain points (poles) is obtained only if the potential is in the shape of a well, with one or several surrounding barriers (Figure 18). Indeed, consider a well with one barrier. The wave function in this case is

$$\chi_k(r) = \begin{cases} A(k)\,\chi_k^{(0)}(r) & \text{for } r < R_1; \\ \alpha(k)\,\chi^{(+)}(r) + \beta(k)\,\chi^{(-)}(r) & \text{for } R_1 < r < R, \\ \sqrt{\frac{2}{\pi}}\sin(kr + \delta) & \text{for } r > R. \end{cases} \tag{27.9}$$

Here $\chi_k^{(0)}$ is the regular (at the origin) solution of the Sch. Eq. in region I; $A(k)$, $\alpha(k)$, and $\beta(k)$ are completely determined by matching the solutions at the boundaries of the different regions. To be specific, we normalize $\chi_k^{(0)}$

as in (27.5). The functions $\chi^{(-)}$ and $\chi^{(+)}$ are two independent solutions of the Sch. Eq. under the barrier (region II). Both these solutions are monotonic, but one decreases and the other increases with increasing r. Qualitatively their behavior is described in the quasiclassical approximation by the expressions

$$\chi^{(\pm)}(r) = \exp\left\{\pm \int_{R_1}^{r} |k|\, dr\right\}; \quad k = \sqrt{\frac{2m}{\hbar^2}(E-U)}\,. \tag{27.10}$$

If the potential barrier is sufficiently wide and high, i.e., if $\int_{R_1}^{R} |k|\, dr \gg 1$, the two functions are essentially different from one another for $r \sim R$, even though they are equal for $r = R_1$ ($\chi^{(\pm)}(R_1) = 1$) (Figure 19):

$$\chi^{(+)}(R) \gg \chi^{(-)}(R). \tag{27.11}$$

The functions $\chi_k^{(0)}$ and $\chi_k^{(\pm)}$ are not particularly sensitive to k, since k enters only through the intermediacy of the term $(E-U)$ in the Sch. Eq., which varies insignificantly for small changes in E. Matching of these functions, however, may give rise to very pronounced energy dependence. Indeed let α and β, as determined by the matching conditions, be fairly close to each other (the exact criteria will be derived below). In this case, on account of (27.11), the interior wave function is approximately equal to $\alpha\chi^{(+)}(R)$ for $r = R$ and its logarithmic derivative hardly depends on energy (since $\chi^{(+)}$ itself is not very sensitive to k). The phase $\delta(k)$ is thus also insensitive to energy, and the wave function $\chi(r)$ has the form shown schematically in Figure 20. It is significant that the wave function retains this form in a wide range of α and β values. The necessary criterion for this state of affairs is clearly

$$\left|\frac{\alpha}{\beta}\right| > \frac{\chi^{(-)}(R)}{\chi^{(+)}(R)} = \exp\left\{-2\int_{R_1}^{R} |k|\, dr\right\}. \tag{27.12}$$

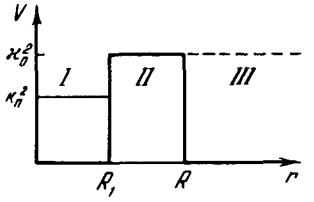

FIGURE 18.

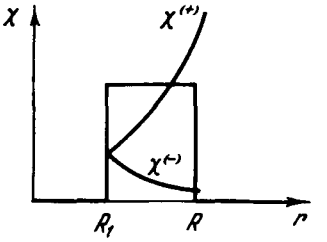

FIGURE 19.

The situation changes radically near the points where $\alpha(k)$ vanishes. Indeed, at these points, the wave function under the barrier monotonically decreases, $\chi_k(r) = \beta\chi_k^{(-)}(r)$, and $\chi_k(r)$ has the form schematically shown in Figure 21. Thus, near the points $k = k_l$, where α vanishes, the wave function abruptly changes passing through all the intermediate stages between the cases depicted in Figures 20 and 21. It is clear that the energy dependence

becomes more pronounced as the ratio $\chi^{(-)}(R)/\chi^{(+)}(R)$ increases, i.e., as the potential barrier becomes wider and higher. If there is no barrier, the situation described here cannot arise, since $\chi^{(+)}(R)$ and $\chi^{(-)}(R)$ will always be of the same order of magnitude.

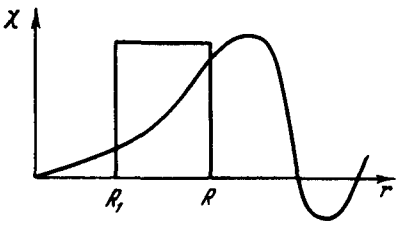

FIGURE 20.

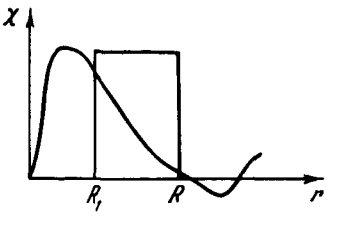

FIGURE 21.

§ 28. EXAMPLE OF A QUASISTATIONARY STATE

We will now investigate a particular example of a potential (see Figure 18) in which a particle has a quasistationary state.

For $r < R_1$ or $r > R$ the Sch. Eq.

$$\chi_k'' + k^2\chi_k = 0$$

has two independent solutions $e^{\pm ikr}$. For $R_1 < r < R$

$$\chi_k'' - \varkappa^2\chi_k = 0, \quad \text{where } \varkappa = \sqrt{\varkappa_0^2 - k^2}, \quad \varkappa_0 = \sqrt{2mV_0}.$$

We will first find a solution which has the form e^{ikr} at infinity. It is sought in the form

$$\chi_k^{(+)}(r) = \begin{cases} e^{ikr} & \text{for } r > R, \\ ae^{\varkappa r} + \beta e^{-\varkappa r} & \text{for } R > r > R_1, \\ ae^{ikr} + be^{-ikr} & \text{for } r < R_1. \end{cases} \tag{28.1}$$

Matching these expressions at the boundaries of the different regions, we obtain for the coefficients

$$\left.\begin{aligned} \alpha &= \frac{1}{2}\left(1 + i\frac{k}{\varkappa}\right)e^{ikR - \varkappa R}, \\ \beta &= \frac{1}{2}\left(1 - i\frac{k}{\varkappa}\right)e^{ikR + \varkappa R}, \\ a &= \frac{\varkappa}{4ik}e^{ik(R-R_1)+\varkappa\rho}\left\{\left(1 + i\frac{k}{\varkappa}\right)^2 e^{-2\varkappa\rho} - \left(1 - i\frac{k}{\varkappa}\right)^2\right\}, \\ b &= \frac{\varkappa}{4ik}e^{ik(R+R_1)+\varkappa\rho}\left\{\left(1 - e^{-2\varkappa\rho}\right)\left(1 + \frac{k^2}{\varkappa^2}\right)\right\}, \end{aligned}\right\} \tag{28.2}$$

where $\rho \equiv R - R_1$. Taking the complex conjugate of $\chi^{(+)}(r)$, we obtain the second independent solution

$$\chi_k^{(-)}(r) = \chi_k^{(+)*}(r) \sim e^{-ikr} \text{ for } r > R. \tag{28.3}$$

The general solution is written as

$$\chi_k(r) = \sqrt{\frac{2}{\pi}} S^{-1/2} \frac{1}{2i} (-\chi_k^{(-)} + S\chi_k^{(+)}) \sim \sqrt{\frac{2}{\pi}} \sin(kr+\delta). \tag{28.4}$$

In the interior region, by (28.1), this function is

$$\chi_k(r) = -\sqrt{\frac{2}{\pi}} S^{-1/2} \frac{1}{2} \left\{ \frac{1}{i} [(a+b)^* - S(a+b)] \cos kr + \right.$$
$$\left. + [(b-a)^* + S(b-a)] \sin kr \right\}. \tag{28.5}$$

To make this function regular at the origin, the coefficient before the cosine should vanish. Using this condition and (28.2), we thus find the scattering matrix:

$$S(k) = e^{2i\delta} = \frac{a^* + b^*}{a+b} = e^{-2ikR} \frac{\varkappa - ik}{\varkappa + ik} \frac{e^{-2\varkappa\rho} + \frac{\varkappa + ik}{\varkappa - ik} \zeta(k)}{e^{-2\varkappa\rho} + \frac{\varkappa - ik}{\varkappa + ik} \zeta(k)}, \tag{28.6}$$

where

$$\zeta(k) = \frac{k \cot kR_1 + \varkappa}{k \cot kR_1 - \varkappa}.$$

If the barrier is sufficiently high and wide, so that $\varkappa\rho \gg 1$, $e^{-2\varkappa\rho}$ is very small, and dropping it in (28.6) we obtain

$$S(k) = e^{-2ikR} \frac{\varkappa + ik}{\varkappa - ik}. \tag{28.7}$$

Omission of $e^{-2\varkappa\rho}$ in expression (28.6) for $S(k)$ is permissible everywhere except near the point $k = k_n$ where $\zeta(k)$ vanishes. Let us investigate this neighborhood. Expanding $\zeta(k)$ in powers of $(k - k_n)$, we write

$$\zeta(k) = \frac{k - k_n}{2k_n} \left[1 + \left(\frac{k_n}{\varkappa_n} \right)^2 \right] (1 + \varkappa_n R_1); \quad \varkappa_n = \sqrt{\varkappa_0^2 - k_n^2}. \tag{28.8}$$

The denominator in (28.6) is thus equal to

$$e^{-2\varkappa\rho} + \frac{\varkappa_n - ik_n}{\varkappa_n + ik_n} \left[1 + \left(\frac{k_n}{\varkappa_n} \right)^2 \right] (1 + \varkappa_n R_1) \frac{k - k_n}{2k_n} \tag{28.9}$$

and therefore vanishes for $k = k_0$:

$$k_0 = k_n - e^{-2\varkappa\rho} \frac{2k_n \varkappa_n^2 (\varkappa_n + ik_n)^2}{(\varkappa_n^2 + k_n^2)^2 (1 + \varkappa_n R_1)} \equiv k_1 - ik_2. \tag{28.10}$$

$S(k)$ thus has a pole at $k = k_0$; we see from the expression for k_0 that this pole is located in the lower halfplane. Using (28.9), (28.10), we write $S(k)$ near the pole in the form

$$S(k) \equiv e^{-2ikR} \frac{\varkappa + ik}{\varkappa - ik} \frac{k + k_0^*}{k - k_0}. \tag{28.11}$$

In the immediate neighborhood of the pole, the first two factors can be treated as constant, putting

$$e^{2i\varphi} = e^{-2ik_1R}\frac{\varkappa + ik_1}{\varkappa - ik_1}. \tag{28.12}$$

Changing over from wave vectors to energies, we write S in the form

$$S(E) = e^{2i\varphi}\frac{E - E_0 - i\Gamma/2}{E - E_0 + i\Gamma/2}, \tag{28.13}$$

where the resonance energy E_0 and the resonance width Γ are ($e^{-2\varkappa\rho} \ll 1$)

$$E_0 = \frac{\hbar^2 k_n^2}{2m}; \quad \Gamma = 16E_0 e^{-2\varkappa\rho}\frac{\varkappa_n^3 k_n}{(\varkappa_n^2 + k_n^2)^2(1 + \varkappa_n R_1)}. \tag{28.14}$$

It would be very enlightening to consider the physical origin of the quasistationary states. Let the right-hand wall R of the potential barrier extend to infinity. In this case the pole k_0 approaches k_n and in the limit we end up with a potential shown in Figure 18 by the dashed line. Clearly the spectrum for $k < \varkappa_0$ with this potential is a discrete spectrum. All states vanish, except the one at $k = k_n$, when

$$k_n \cot k_n R_1 + \varkappa_n = 0,$$

and the wave function falls off at infinity as $e^{-\varkappa_n r}$. Thus, in the limit as $R \to \infty$, the quasistationary state is replaced by a true stationary state.

Let now R be a large but finite number. In this case the true stationary state cannot exist, so that particles from the interior region $r < R$ will tunnel through the barrier and escape to infinity. The stationary state is thus replaced by a quasistationary state. Since the probability of this "tunneling" for large $\varkappa\rho$ is very low, the decay time T is extremely high. Clearly, if we are concerned with short times, when the decay probability is ignorable, the unstable state may be treated as an ordinary stable state. In other words, a "quasistationary" state is defined as a state which replaces the stationary state when a finite decay probability has to be considered.

Using the argument of the previous section, we can readily estimate the lifetime T:

$$T \approx T_0\frac{\Gamma^2/4}{(E - E_0)^2 + \Gamma^2/4}; \quad T_0 = \frac{2\hbar}{\Gamma}.$$

Physically we can speak of a quasistationary state only if T is greater than the free time of flight $\tau = \frac{R}{v_0}$. This condition is met in a certain energy range ΔE around E. Taking $T_0/\tau \gg 1$, we obtain in an elementary way

$$|\Delta E| \lesssim \frac{\Gamma}{2}\sqrt{\frac{T_0}{\tau}}.$$

Hence it is clear that the concept of a "quasistationary state" is not rigorously defined. The only condition for the formation of a relatively long-lived state during the scattering of particles by a potential barrier

is that the particle energy differ from E_0 by not more than ΔE. It is in this sense that we say that a quasistationary state of width Γ has no fixed energy and is "spread" over a certain energy interval $\sim \Gamma \sqrt{T_0/\tau} > \Gamma$.

As an illustration, consider the following example. Suppose that besides a quasistationary state of energy E_0 and width Γ there is also a bound state of energy E_1. Consider a process in which a particle of energy E is scattered by this potential and emits a γ quantum, dropping to a bound state with energy E_1 (radiative capture). The probability $w(E)$ is determined as always by the square of the matrix element

$$w(E) \sim |(\chi_E, \hat{O}\chi_1)|^2,$$

where $\hat{O}$ is the electromagnetic transition operator and χ_1 is the wave function of the bound state, which differs from zero only in a small neighborhood of the potential. Therefore the energy dependence of $w(E)$ is mainly determined by $\overline{\chi_E^2}$:

$$w(E) = \text{const} \cdot \overline{\chi_E^2} \approx \text{const} \cdot \frac{\Gamma^2/4}{(E - E_0)^2 + \Gamma^2/4}.$$

If the scattered beam is monochromatic, monochromatic γ quanta of energy $E - E_1$ are emitted. However, the probability of γ quantum emission, as we see from the above relation, is highly sensitive to particle energy. $w(E)$ is high only when E is close to E_0.

Now suppose that the incident beam contains particles of various energies E spread within an interval $\Delta E \gg \Gamma$. Radiative capture operates only for particles having energies close to E_0. Correspondingly the energy of the γ quanta will be close to $E_0 - E_1$, and their spectrum will have the schematic form of the curve shown in Figure 22. The width of the resonance curve is determined by the shape of the $w(E)$ curve and is equal to Γ.

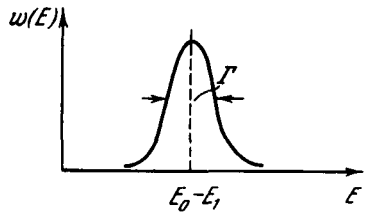

FIGURE 22.

The width of the γ quanta spectrum is thus determined by two factors: the energy spread ΔE in the incident beam and the width Γ of the resonance level. For $\Delta E = 0$ all quanta have the same energy $E - E_1$. As ΔE increases from zero to Γ, the scatter in the energy of the Γ quanta also increases. As ΔE is further increased, however, the energy spread of the emitted quanta remains invariably of the order Γ. Thus for $\Gamma \to 0$ the quanta can always be treated as monochromatic, irrespective of the beam energy spread ΔE. It seems as if the scattered particles are first trapped by a virtually stable state with energy E_0 and then drop to a lower state χ_1 emitting a quantum.

For small but finite Γ, the quasistationary state is said not to have a definite energy. Note that in every particular instance a state with fixed energy E, equal to the energy of the incident particle, is formed. The energy uncertainty of the quasistationary state is to be understood only in the sense that for any energy value E from the interval $|E - E_0| \lesssim \Gamma$ a relatively long-lived state may form.

We have derived a number of general formulas for quasistationary states. In their derivation we used only the energy dependence of the wave function associated with the pole term in $S(k)$. All the other quantities were treated as constant. If we are concerned with the energy range not too near the pole ($|E - E_0| > \Gamma$), this procedure is not very reliable and the actual form of the potential should be taken into consideration in calculating the energy dependence of all the physical quantities. In other words, in these cases we can no longer introduce the general concept of a "quasistationary state" which depends on the potential through E_0 and Γ only. There is no fixed boundary between real "quasistationary" states and states which are essentially dependent on the form of the potential. Various authors draw this boundary in various places depending on their personal tastes and needs. Often the position of this boundary is decided by the particular author's wish to interpret the experimental data as supporting one of the several theoretical alternatives.

To avoid confusion, note that when we say anything about a "quasistationary" state, we mean that the assertion is entirely true only in the limit as $\Gamma \to 0$.

§ 29. THE DECAY OF A QUASISTATIONARY STATE

We have seen that rigorous treatment of quasistationary states is impossible without taking into consideration the particular physical process leading to the formation of the state. If we are dealing, say, with potential scattering of particles with formation of a "quasistationary" intermediate state, the process is described by the function $\chi_k(r)$ introduced in the previous section in connection with scattering problems. The "quasistationarity" emerges here only as an exceptionally large value of the wave function inside the barrier. Quasistationary states produced by various reactions also have their own specific wave functions. Finally we can consider the problem of the decay of a quasistationary state.* In this case we again will be dealing with a characteristic wave function. In the present section we will derive this function and try to analyze its properties. In doing so, we follow Drukarev's method /173/.

The problem is formulated as follows. Consider a potential barrier (of the form depicted in Figure 18). At the time $t = 0$ the wave function inside the barrier is $\chi_0(r)$; it is zero under the barrier and elsewhere. We are interested in finding the evolution of the wave function in time, i.e., the function $\chi(r, t)$ for $t > 0$. This is a nonstationary problem and to solve it we naturally need the time-dependent Sch. Eq.

$$i\hbar\dot{\chi} = -\frac{\hbar^2}{2m}\chi'' + U\chi \tag{29.1}$$

with the initial condition $\chi|_{t=0} = \chi_0$. The wave function is further required to remain bounded for all r and t. Following the usual technique, we seek $\chi(r, t)$ in the form of an expansion

$$\chi(r, t) = \int_0^\infty dkc(k)\chi_k(r)e^{-i\frac{Et}{\hbar}}, \tag{29.2}$$

* Various aspects of the decay of a quasistationary state are considered in /173–177/.

where $\chi_k(r)$ are the solutions of the time-independent equation

$$-\frac{\hbar^2}{2m}\chi_k'' + U\chi_k = E\chi_k,$$

normalized to $\delta(k - k_1)$. These solutions outside the range of the potential have the standard form

$$\chi_k = \sqrt{\frac{2}{\pi}}\sin(kr + \delta(k)) = \sqrt{\frac{2}{\pi}}\frac{1}{2i}(S^{1/2}(k)\,e^{ikr} - S^{-1/2}(k)\,e^{-ikr}). \tag{29.3}$$

The function $c(k)$ in (29.2) is found from the initial condition:

$$c(k) = \int_0^\infty dr\chi_0\chi_k. \tag{29.4}$$

The dependence of $c(k)$ on k should clearly be the same as for the wave function χ_k. Thus, $c(k)$ is representable in the form (compare with (29.3))

$$c(k) = \frac{1}{i}(\alpha(ik)S^{1/2}(k) - \alpha(-ik)S^{-1/2}(k)), \tag{29.5}$$

where $\alpha(ik)$ is some smooth function of k. The above expressions show that the integrand in (29.2) is an even function of k. Using this fact, we write (29.2) in the form

$$\chi(r, t) = -\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\,[\alpha(ik)S(k) - \alpha(-ik)]\,e^{ikr - \frac{iEt}{\hbar}} \tag{29.6}$$

We now introduce a new variable

$$y = \sqrt{\frac{i\hbar t}{2m}}\left(k - \frac{mr}{\hbar t}\right). \tag{29.7}$$

Substituting this variable in (29.6), we obtain

$$\chi(r, t) = B\int_{-\sqrt{i}\infty}^{\sqrt{i}\infty} dy\,e^{-y^2}[\alpha(ik(y))S(k(y)) - \alpha(-ik(y))], \quad B \equiv -\sqrt{\frac{m}{i\pi\hbar t}}e^{\frac{imr^2}{2\hbar t}}. \tag{29.8}$$

The integration path in this integral (Figure 23) is an unsuccessful choice, since everywhere along this line e^{-y^2} is an oscillating function. We therefore rotate the integration path so that it coincides with the real axis. e^{-y^2} now rapidly falls off in the direction of both positive and negative y.

The functions α are smooth and without any singularities, so that they do not interfere with this deformation of the integration path. The situation, however, is different as far as $S(k)$ is concerned, since we definitely know that this function has singularities. Let us find their position in the complex plane.

The most general expression for $S(k)$ in the case of a single quasi-stationary state is (see (27.2))

$$S(k) = S_0(k)\frac{(k - k_0^*)(k + k_0)}{(k - k_0)(k + k_0^*)}.$$

Here $S_0(k)$ is some smooth function of k, k_0 is the pole. Changing over to a new variable y, we find

$$S(k(y))=S_0(k(y))\frac{\left(y+\sqrt{\frac{i\hbar t}{2m}}\left(\frac{mr}{\hbar t}-k_0^*\right)\right)\left(y+\sqrt{\frac{i\hbar t}{2m}}\left(\frac{mr}{\hbar t}+k_0\right)\right)}{\left(y+\sqrt{\frac{i\hbar t}{2m}}\left(\frac{mr}{\hbar t}-k_0\right)\right)\left(y+\sqrt{\frac{i\hbar t}{2m}}\left(\frac{mr}{\hbar t}+k_0^*\right)\right)}. \tag{29.9}$$

We should distinguish between two cases.

(1) $r > v_r t$, where v_r is the velocity corresponding to resonance energy, $v_r = \frac{\hbar k_1}{m}$, k_1 is the real part of k_0, $k_0 \equiv k_1 - ik_2$. In this case the poles of $S(k(y))$ lie in the diagonally hatched regions in Figure 23 and do not interfere with the rotation of the integration contour toward the real axis. As the integrand in (29.8) contains the exponential function e^{-y^2}, the main contribution to the integral comes from the region $y \approx 0$ and we approximately get

$$\chi_n(r, t) = B\sqrt{\pi}S^{1/2}(k(0))\, ic(k(0)), \tag{29.10}$$

where the subscript n refers to the nonresonant case. Here $S(k)$ and $c(k)$ should be taken for the value of k corresponding to $y = 0$, i.e., $k(0) = \frac{mr}{\hbar t}$. Thus $k(0)$ is the value of the wave vector k which characterizes the particle emitted at the time $t = 0$ from the origin and reaching the point r at time t.

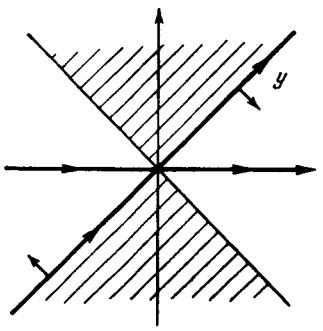

FIGURE 23.

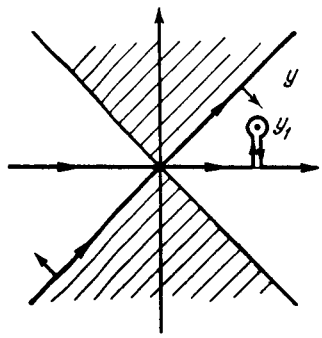

FIGURE 24.

We see from (29.10) that the function $\chi_n(r, t)$ is entirely determined by the coefficient $c(k(0))$, which specifies the fraction of the initial state corresponding to particles of wave vector $k(0)$. Thus, χ_n describes particles which left the origin at time $t = 0$, i.e., immediately after the formation of the initial state χ_0. Physically this means that particles with this k leave the region of nonzero potential instantaneously, without lingering there.

A more complex situation arises in the second case:

(2) $r < v_r t$. In this case r and t are such that at the point r we can observe both fast particles with $v > v_r$ and slow particles with $v \leqslant v_r$. We see from (29.9) that the poles of $S(k(y))$ in this case are located so that one

of them obstructs the rotation of the integration contour toward the real axis. This is the pole situated in the unhatched region of Figure 24 at the point

$$y_1 = \sqrt{\frac{i\hbar t}{2m}}\left(\frac{m}{\hbar}\left(v_r - \frac{r}{t}\right) - ik_2\right).$$

Thus in calculating the integral (29.6), we obtain two terms: one contribution comes from the region $y = 0$ and the resulting term is entirely analogous to χ_n in (29.10); the second contribution comes from the pole. The final result is

$$\left.\begin{aligned} \chi(r, t) &= \chi_n(r, t) + \chi_r(r, t), \\ \chi_r(r, t) &= -2\pi i B\alpha(ik_0)\, e^{-y_1^2}\operatorname{Res} S(k(y_1)). \end{aligned}\right\} \tag{29.11}$$

The first term χ_n has the same meaning as before. It corresponds to particles of velocity $v = \frac{r}{t}$ instantaneously escaping outside the potential range.

The second term is much more interesting. Although the pole $y = y_1$ lies far from the real axis, it gives a substantial contribution to the integral, and the second term may thus be much larger than the first term. This is so because e^{-y^2} is definitely not small at the pole. Reverting from y to the original variable k, we write the additional term in (29.11) in the form

$$\chi_r(r, t) = \sqrt{2\pi}\,\alpha(ik_0)\, S_0(k_0)\,\frac{\Gamma}{2\hbar v_r}\, e^{ik_1 r - \frac{iE_0 t}{\hbar} - \frac{\Gamma}{2\hbar}\left(t - \frac{r}{v_r}\right)}. \tag{29.12}$$

All the smooth functions are taken at the point $k = k_0$, i.e., at the pole corresponding to a quasistationary state; χ_r describes a traveling wave whose front propagates with a velocity v_r.

Let us estimate the coefficients $c(k)$ and $\alpha(ik_0)$ entering χ_n and χ_r. For $c(k)$ we have

$$c(k) = \int_0^R \chi_0 \chi_k\, dr \sim \bar{\chi}_0 R \tag{29.13}$$

(R is the range of the potential). To obtain an estimate for $\alpha(ik_0)$, note that for $k \approx k_0$, the function χ_k may be written in the form $A(k)\,\chi^{(0)}(r)$, where $\chi^{(0)}$ is normalized to unity (see (27.5)) and $A^2(k)$ has a pole at the point $k = k_0$ (see (27.7)). We thus have a chain of equalities

$$c(k) = \frac{1}{i}\left(\alpha(ik) S^{1/2}(k) - \alpha(-ik) S^{-1/2}(k)\right) \sim A\int_0^R \chi_0 \chi^{(0)}\, dr \sim A\bar{\chi}_0\sqrt{R}.$$

Since for $k \to k_0$, $S^{-1}(k) \to 0$, we have

$$\alpha(ik_0) = i\bar{\chi}_0\sqrt{R}\lim_{k\to k_0} S^{-1/2}(k)\, A(k) = -\bar{\chi}_0\sqrt{R} S_0^{-1/2}(k)\sqrt{\frac{\hbar v_r}{2\pi\Gamma}}. \tag{29.14}$$

Note that there is a definite analogy between $c(k)$ and $\alpha(ik_0)$. To illustrate this point, consider the solution

$$\tilde{\chi}_k(r) = 2i\sqrt{\frac{\pi}{2}}\, S^{-1/2}\chi_k(r) \sim e^{ikr} - S^{-1}(k)\, e^{-ikr},$$

which for $k \to k_0$ reduces to the solution χ_r corresponding to a complex energy eigenvalue $E_0 - \frac{i\Gamma}{2}$ with the asymptotic behavior of $e^{ik_0 r}$. The corresponding overlap integral $\tilde{c}$ is

$$\tilde{c} = \int \tilde{\chi}_k \chi_0 \, dr = i \sqrt{2\pi} \, S^{-1/2} c(k) = \sqrt{2\pi} \, (\alpha(ik) - \alpha(-ik) S^{-1}(k)).$$

Taking the limit as $k \to k_0$, we find

$$\alpha(ik_0) = \frac{1}{\sqrt{2\pi}} \int \chi_r \chi_0 dr. \tag{29.15}$$

Thus $c(k)$ and $\alpha(ik_0)$ are both overlap integrals with χ_0, although different functions are involved in the two cases: $c(k)$ corresponds to functions with real E and $\alpha(ik_0)$ to functions with complex energy eigenvalue.

In analyzing (29.10)—(29.15) we should remember under what conditions they were derived: in taking the integral in (29.8) the integrand (with the exception of e^{-y^2}) was assumed to be relatively insensitive to y for $y \sim 0$. This is true if all the factors in the integrand in (29.8) do not change much when y is incremented by unity.

A change of y by $\Delta y \sim 1$ corresponds to

$$\Delta k \sim \left(\frac{2m}{\hbar t}\right)^{1/2}.$$

The treatment is legitimate if Δk is less than the interval δk where $S(k)$ and $\alpha(ik)$ may be regarded as constant.

In nuclear physics, a characteristic nonuniformity length is 1 keV, and the energy is of the order of 1 MeV; we have

$$\delta k = \frac{\delta E}{\hbar} \sqrt{\frac{m}{2E}}.$$

Hence we obtain the time t starting with which $\Delta k < \delta k$:

$$t > \frac{4E\hbar}{(\delta E)^2} = \frac{10^{-6} \cdot 10^{-27}}{10^{-24}} = 10^{-15} \text{ sec}.$$

In atomic effects, $\delta E \sim 0.1$ eV, $E \sim 10$ eV, so that

$$t > \frac{10^{-11} \cdot 10^{-27}}{10^{-26}} = 10^{-12} \text{ sec}.$$

In elementary particle physics $\delta E \sim 10$ MeV, $E \sim 1000$ MeV, so that

$$t > \frac{10^{-8} \cdot 10^{-27}}{10^{-20}} = 10^{-20} \text{ sec}.$$

These estimates show that expressions (29.10)—(29.14) are valid for virtually all measurable times. It is only at the very first instants following the start of decay that these expressions do not apply.

§ 30. RADIOACTIVE DECAY

The physical meaning of the various expressions in the previous section is perfectly clear: at the time $t = 0$ the wave function $\psi_0(r)$ did not correspond to a state with definite energy. The probability of finding the particle with energy E (and wave vector k) is proportional, by the general postulates of quantum mechanics, to the square of the matrix element $\langle 0|k\rangle = \int \psi_0^* \psi_k dr$. Therefore, from the standpoint of elementary physics, the "spreading" of the initial state can be described as follows: if the particle with energy E does not linger inside the potential barrier and escapes instantaneously, it will reach the point $r = vt$ after the time t. This is precisely the meaning of (29.10) and of the first term in (29.11): the amplitude of the wave function at the point r is proportional to the amplitude of the state with energy E (and corresponding velocity $v = \frac{\hbar k}{m}$) in the initial wave function.

If now E is close to the energy E_0 of the quasistationary state, elementary kinematic considerations lead us to expect that no such particles will yet be observed for $r > v_0 t$: none of them could have reached these points by that time. If $r < v_0 t$, however, these particles should be observed for all r, since if a state has a certain lifetime τ, these particles are observed not only at the point $r = v_0 t$ but also at the point $r = v_0 (t - \tau)$. If there is a probability $P(\tau)$ that the particle has a lifetime τ, the particle density (at a distance r from the source at time t) should be proportional to $P(\tau - \frac{r}{v_0})$. This is in fact the case represented by the second, resonance term in (29.11). Moreover, from the form of this term we conclude that for $E \sim E_0$ a "quasistationary" state is formed, and the probability of its decay at time τ after formation is proportional to $e^{-\frac{\Gamma\tau}{\hbar}}$. We thus arrive at the well-known law of radioactive decay. The probability density distribution of particles $|\psi(r, t)|^2$ at time t has the form shown in Figure 25. The maximum at small r corresponds to the region inside the barrier, and the maximum at large r corresponds to decay of a "quasistationary" state at $t = 0$, instantaneously after its formation; this peak advances with velocity v_0. Owing to continued decay, the particle density in the quasistationary state gradually decreases. To the right, i.e., for $r > v_0 t$, the probability density is less, since the "decay" products have not yet reached that region. The finite "background" of particles for $r > v_0 t$ is associated with the wide range of particle energies present in the initial state.

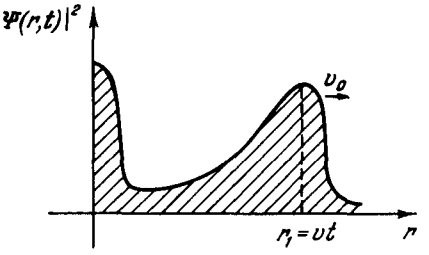

FIGURE 25.

Note that in the stationary theory the wave function of a quasistationary state is generally adopted as the solution $\varphi_{k_0}(r, t)$ of the Sch. Eq. which satisfies the boundary condition at $r = 0$ and behaves as $e^{ik_0 r - i(E_0 - \frac{i\Gamma}{2})t}$ (k_0 is a complex number) for $r \to \infty$. On the other hand, for real k, we have the wave function of the scattering problem, whose asymptotic expression is

$$\chi_k(r)\, e^{-\frac{iEt}{\hbar}} \sim \frac{1}{2i}\sqrt{\frac{2}{\pi}}\left(e^{ikr} S^{l/2}(k) - e^{-ikr} S^{-l/2}(k)\right) e^{-\frac{iEt}{\hbar}}. \qquad (30.1)$$

A quasistationary state corresponds to a pole of $S(k)$. Dividing $\chi_k(r)$ by $\frac{1}{i\sqrt{2\pi}} S^{1/2}(k)$ we find that for $k \to k_0$ the second term vanishes and

$$\frac{i\sqrt{2\pi}}{S^{1/2}(k)} \chi_k(r) e^{-\frac{iEt}{\hbar}} \xrightarrow[k \to k_0]{} \varphi_{k_0}(r, t). \tag{30.2}$$

Thus the two solutions are intimately linked with one another. The advantage gained from the introduction of the function φ_{k_0} is obvious. First, the k_0 for which the Sch. Eq. has a solution of the form φ_{k_0} directly determines the position and the width of the quasistationary state. Moreover, comparison of (30.2) with (29.12) shows that φ_{k_0} for $r < v_0 t$ faithfully reproduces the dependence of the true wave function $\psi(r, t)$ of the decaying state on r and t (here t is reckoned from the time of formation of the decaying state).

The problem of the allegedly exponential character of radioactive decay is often discussed in the literature /178–180/. In this connection we wish to make the following remarks. From expression (29.11) of the previous section we see that $|\psi(r, t)|^2$ is a nonexponential (decreasing) function of time. This is understandable, since by specifying an arbitrary initial state $\psi_0(r)$, we form a superposition of an exponentially decaying quasistationary state and a packet of particles with a continuous spectrum, which in fact introduce the first nonexponential term in (29.11).* This is a physical inevitability.

If the resonance term is the dominant term in $\psi(r, t)$ (which is almost always the case), the decay is exponential. That the resonance term is almost always dominant can be easily verified. Using the expressions of this chapter, we readily estimate the ratio of the squares of the moduli of the first and second term in the wave function (29.11) for $r \ll v_0 t$. To orders of magnitude we have

$$\rho \equiv \left|\frac{\psi_n}{\psi_r}\right|^2 \sim \frac{\hbar}{E_0 t} e^{\Gamma t/\hbar} = \frac{\Gamma}{E_0} \frac{t_0}{t} e^{t/t_0}, \quad t_0 = \frac{\hbar}{\Gamma}. \tag{30.3}$$

The dependence of this ratio on t/t_0 is schematically shown in Figure 26. It is clear from the figure that the nonresonant term is greater than the resonance term of the wave function only for very small ($t < t_1$) or very large ($t > t_2$) times. For t_1 and t_2 we have approximately

$$\left.\begin{aligned} t_1 &\approx t_0 \frac{\Gamma}{E_0}; \\ t_2 &\approx t_0 \ln \frac{E_0}{\Gamma}. \end{aligned}\right\} \tag{30.4}$$

For intermediate t values, the resonance term dominates. This means that for all t between the limits $t_1 < t < t_2$ the decay is practically exponential.

In the particular case of alpha decay $E_0 \approx 1$ MeV $\approx 10^{-6}$ erg, $t_0 \gtrsim 1$ sec, $\Gamma \leqslant 10^{-15}$ eV $\approx 10^{-27}$ erg. Hence

$$t_1/t_0 \sim 10^{-21}; \quad t_2/t_0 \sim 50. \tag{30.5}$$

* When a complete system of stationary states is used, the nonexponential character of decay follows from the Krylov–Fock theorem /181/ (which states that the decay law is completely determined by the energy spectrum of the initial state), since the energy spectrum of the initial state is bounded from below.

We see from these estimates that alpha decay follows the exponential curve with astonishing accuracy. Deviations from the exponential law can be observed only at the very first instant following the formation of the decaying state or for very large times ($t > 50t_0$), when virtually no decaying element has been left ($e^{-50} \approx 10^{-20}$).

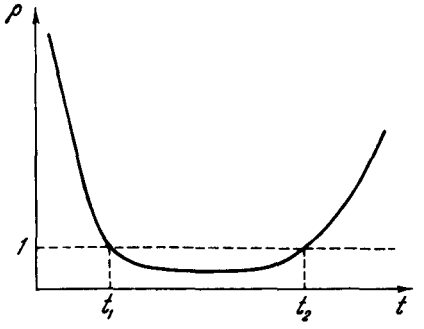

FIGURE 26.

The radioactive decay is thus seen to be exponential if the resonance width Γ is sufficiently small ($\Gamma \ll E_0$). In nuclear physics E_0 is of the order of 1 MeV and to ensure exponential decay we should have $\Gamma \ll 1$ MeV. In elementary particle physics $E_0 \sim 100 - 1000$ MeV. In atomic physics $E_0 \sim 10$ eV. In these cases we respectively have $\Gamma \ll 100 - 1000$ MeV and $\Gamma \ll 10$ eV.

We should always remember, however, that the preceding treatment is based on one highly significant assumption. In deriving the relations of the previous section we assumed that $\langle 0|k\rangle = \int \psi_0^* \psi_k dr$, S_0, and α did not depend much on k. This is not always so. We can create a wave packet with energy spread

$$\Delta E \ll \Gamma$$

and mean energy $\bar{E}$ lying somewhere in the interval $[E_0 - \Gamma, E_0 + \Gamma]$. In this case, all the quantities of the form S_0, α will be highly variable in the region around $\bar{E}$ and a direct calculation will show, as in the previous section, that the decay has nothing in common with the exponential function.

In other words, we may say that for $\Delta E \gg \Gamma$ the probability of formation of a quasistationary state with energy E is independent of ΔE and is given by

$$w(E) \sim \frac{\Gamma/2}{(E - E_0)^2 + \Gamma^2/4}$$

(this is known as a Lorentz distribution).

If the probability distribution is not a Lorentz distribution, the decay is not exponential. This case is readily realized in practice. Consider an atom in the second excited state, whose width Γ_2 is much less than the width Γ_1 of the first excited state. Suppose that a cascade gamma transition is allowed: the system emits a quantum γ_2 (of energy $\hbar\omega_2$) and drops to the first excited level; then it emits a quantum γ_1 (of energy $\hbar\omega_1$) and drops to the ground state. The energy of the quantum γ_2 can be measured; $\hbar\omega_2$ is measurable by modern techniques with an accuracy $\Delta(\hbar\omega_2) \ll \Gamma_1$. The first excited level, however, is not populated according to the Lorentz curve: only a certain part of the level is filled. The decay of the first level thus is not an exponential function of time.

If, however, $\Gamma_2 \gg \Gamma_1$ and the second level is completely filled (i.e., in the entire energy interval $\Delta E \sim \Gamma_2$), the first level is always populated according to the Lorentz curve and therefore decays exponentially.

§ 31. PERTURBATION THEORY FOR QUASISTATIONARY STATES

We have so far mainly concentrated on specific decay properties of quasistationary states. Formally these states constitute a continuum, although on account of their fairly long lifetime they have a number of physical and formal properties which are reminiscent of stationary states. In particular, we can introduce an effective normalization integral for quasistationary states and derive a number of results which are very similar to the corresponding results for stationary states.

In our treatment of the perturbation theory for quasistationary states,* we follow the presentation of /183/.

Suppose that in an unperturbed potential $V(r)$ the particle has a quasistationary state at the point $k_0 = k_1 - ik_2$. We now add a perturbation δV to the potential. How will k_1 and k_2 (i.e., the position E_0 and the width Γ of the resonance) change? This problem can be solved as follows.

The wave function $\chi_k(r)$ is replaced by its logarithmic derivative,

$$z_k(r) = \frac{\chi_k'(r)}{\chi_k(r)}; \quad \chi_k(r) = \exp\left\{\int_0^r z_k(r')dr'\right\}.$$

Using the Sch. Eq., which is satisfied by $\chi_k(r)$, we readily find an equation for z_k:

$$z_k'(r) + z_k^2(r) + (k^2 - V) = 0. \tag{31.1}$$

Since for a state of momentum l the regular function χ_{k_0} behaves for small r as ar^{l+1}, where $a = \text{const}$, we have $z(r) \underset{r\to 0}{\to} \frac{l+1}{r}$ irrespective of the potential. For large r, this solution behaves as e^{ik_0r} and $z(r) \underset{r\to\infty}{\to} ik_0$.

We now introduce a perturbation δV. z_k acquires an increment δz_k and the position of the quasistationary level shifts $k_0 \to k_0 + \delta k_0$. From (31.1) we obtain for δz_k

$$(\delta z_k)' = -2z_k\delta z_k + \delta V - 2k_0\delta k_0. \tag{31.2}$$

Since the limit of $z(r)$ as $r \to 0$ is independent of k, δz_k should satisfy the boundary condition

$$\delta z_k(0) = 0. \tag{31.3}$$

The solution of equation (31.2) satisfying this boundary condition is clearly

$$\delta z_k(r) = \exp\left\{-2\int_0^r z_{k_0}dr\right\}\int_0^r\left\{[\delta V(r') - \right.$$

$$\left. - 2k_0\delta k_0]\exp\left[2\int_0^{r'} z_{k_0}(r'')\,dr''\right]\right\}dr' = \frac{\int_0^r [\delta V(r') - 2k_0\delta k_0]\,\chi_{k_0}^2(r')\,dr'}{\chi_{k_0}^2(r)}. \tag{31.4}$$

For large r, when $\chi_{k_0} \sim Ce^{ik_0r}$, the logarithmic derivative is always equal to ik_0 and $\delta z(\infty) = i\delta k_0$ gives the correction to the energy and the width of the

* This theory was first developed apparently in /182/.

quasistationary state. From (31.4) we have for this case

$$i\,\delta k_0\,(Ce^{ikr})^2 = -2k_0\,\delta k_0 \int_0^r \chi_{k_0}^2(r')\,dr' + \int_0^r \delta V \chi_{k_0}^2(r')\,dr',$$

which may be rewritten as

$$2k_0\,\delta k_0 \equiv \delta k_0^2 = \frac{\int_0^r \chi_{k_0}^2\,\delta V\,dr'}{\int_0^r \chi_{k_0}^2\,dr' - \frac{\chi_{k_0}^2}{2ik_0}}. \tag{31.5}$$

Strictly speaking, this expression is applicable only if V and δV both vanish starting with some $r = K$. It is only in this case that (a) for sufficiently large r, $Ce^{ik_0r} = \chi_{k_0}$, and (b) the upper integration limit can be extended to infinity.

Expression (31.5) is the solution of our problem. The perturbation alters the position and the width of the quasistationary state:

$$E_0 - \frac{i\Gamma}{2} \to \frac{\hbar^2}{2m}(k_0 + \delta k_0)^2.$$

Expression (31.5) is very similar to the general perturbation theoretical expression for level shift. There are only two differences: first it contains the square of the wave functions $\chi_{k_0}^2$ and not the square of the moduli $|\chi_{k_0}|^2$; second, the ordinary formula has the normalization integral $\int_0^\infty |\chi_k|^2 dr$ in the denominator, which is not what we have in (31.5). Note that the integral $\int_0^\infty |\chi_{k_0}|^2 dr$ diverges, since the integrand increases exponentially for $r \to \infty$. The integral $\int_0^\infty \chi_{k_0}^2 dr$ is also meaningless according to the usual definition, but since the integrand increases for $r \to \infty$ while oscillating, we will show how to regularize this integral. It is not sufficient to multiply the integrand by $e^{-\alpha r}$ and let α go to zero. We can show, however, that

$$\lim_{\alpha \to 0} \int_0^\infty \chi_{k_0}^2(r) e^{-\alpha r^2} dr = \int_0^\infty [\chi_{k_0}^2 - (Ce^{ik_0r})^2]\,dr - \frac{C^2}{2ik_0} \tag{31.6}$$

exists, so that the denominator in (31.5) can be treated as a normalization integral of the function χ_{k_0}. *

* Indeed, as is readily seen, the integral is expressible in terms of the error function Φ:

$$\int_0^\infty e^{-\alpha r^2 + 2i(k_1 - ik_2)r}\,dr = \int_0^\infty e^{-\alpha r^2 + 2ik_1 r}(\cos 2k_1 r + i \sin 2k_1 r)\,dr =$$

$$= \frac{1}{2}\sqrt{\frac{\pi}{\alpha}}\left[1 - \Phi\left(-i\frac{k_0}{\sqrt{\alpha}}\right)\right]\exp\left(-\frac{k_0^2}{\alpha}\right).$$

Since $\alpha \to 0$, we may use the asymptotic expansion for Φ:

$$\lim_{\alpha \to 0} \int_0^\infty e^{-\alpha r^2 + 2ik_0 r}\,dr = \frac{1}{2}\sqrt{\frac{\pi}{\alpha}} e^{-\frac{k_0^2}{\alpha}} \frac{1}{\pi} e^{\frac{k_0^2}{\alpha}} \frac{\Gamma\left(\frac{1}{2}\right)\sqrt{\alpha}}{k_0} i = -\frac{1}{2ik_0}.$$

Therefore if we define as the normalization integral the limit

$$\int_0^\infty \chi_{k_0}^2\, dr \equiv \lim_{\alpha\to 0} \int_0^\infty \chi_{k_0}^2\, e^{-\alpha r^2} dr, \tag{31.7}$$

we can rewrite (31.5) in the more familiar form

$$\delta k_0^2 = \frac{\int_0^\infty \delta V \chi_{k_0}^2\, dr}{\int_0^\infty \chi_{k_0}^2\, dr}. \tag{31.8}$$

The above definition of the normalization integral for quasistationary states is quite useful in a number of problems. In the next section we will show, for example, how to apply this technique to the calculation of the coefficient a, which determines the intermediate asymptotic behavior of the wave function.

§ 32. THE ASYMPTOTIC EXPRESSION OF THE WAVE FUNCTION FOR $r \to \infty$ AND $t \to \infty$

This problem was considered before, but then we were mainly interested in the physics of the process. Now we can concentrate on the formal aspects. We will derive an asymptotic expression for the wave function $\psi(r, t)$ for $r \to \infty$ and $t \to \infty$ taking $\psi(r, 0) = \psi_0(r)$.

This problem was solved in /183/ by Laplace's method. We will apply this method to a spherically symmetric problem where the potential $V(r)$, the sought function $\psi(r, t)$, and the initial function $\psi(r, 0)$ depend on r only. We introduce a new function $\psi(r, s)$,

$$\psi(r, s) = -i \int_0^\infty e^{ist} \psi(r, t)\, dt. \tag{32.1}$$

Taking $s = \eta + i\sigma$, we find that

$$\psi(r, s) = -i \int_0^\infty e^{-\sigma t} \psi(r, t)\, e^{i\eta t} dt \equiv \int_{-\infty}^\infty f(r, t) e^{i\eta t} dt, \tag{32.2}$$

i.e., $\psi(r, s)$ is a Fourier transform of the function

$$\left.\begin{aligned} f(r, t) &= 0 && \text{for } t < 0, \\ f(r, t) &= -ie^{-\sigma t}\psi(r, t) && \text{for } t > 0. \end{aligned}\right\} \tag{32.3}$$

On the other hand, for $R < r$,

$$\int_0^r [\chi_{k_0}^2(r) - (Ce^{ik_0 r})^2]\, dr - \frac{C^2}{2ik_0} = \lim_{\alpha\to 0} \int_0^r dr\, [\chi_{k_0}^2(r) - (Ce^{ik_0 r})^2]\, e^{-\alpha r^2} +$$

$$+ \lim_{\alpha\to 0} \int_0^r e^{-\alpha r^2} (Ce^{ik_0 r})^2\, dr = \lim_{\alpha\to 0} \int_0^\infty e^{-\alpha r^2} \chi_{k_0}^2(r)\, dr.$$

We made use of the fact that the cutoff factor $e^{-\alpha r^2}$ in the first integral does not alter the value of the integral for $\alpha \to 0$, as the term in brackets is zero for $r > R$.

Inversion gives f and we find after elementary manipulations

$$\psi(r, t) = -\frac{1}{2\pi i}\int_{-\infty+i\sigma}^{+\infty+i\sigma} \psi(r, s)\, e^{-ist}\, ds. \tag{32.4}$$

The integral in (32.2) exists for f which falls off as $t \to \infty$, i.e., for $\sigma > 0$. However, we will also consider $\psi(r, s)$ for $\sigma < 0$; this can be defined as the analytic continuation of the function $\psi(r, s)$ defined by the integral for $\sigma > 0$.

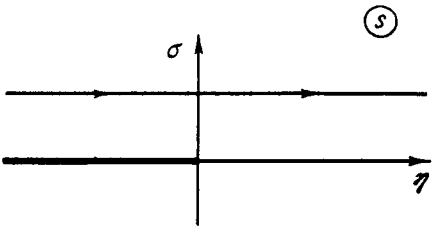

FIGURE 27.

Consider the Sch. Eq.

$$i\hbar\frac{\partial\psi(r, t)}{\partial t} = -\frac{\hbar^2}{2m}\Delta\psi(r, t) + U(r)\,\psi(r, t).$$

Multiplying by $-ie^{ist}$ and integrating with respect to time, we find

$$-\hbar s\psi(r, s) - \frac{\hbar^2}{2m}\Delta\psi(r, s) + U(r)\,\psi(r, s) = -\hbar\psi_0(r). \tag{32.5}$$

Here we assumed that for $r > R$,

$$\lim_{t\to\infty} e^{ist}\psi(r, t) = 0,$$

which implies $\sigma > 0$, i.e., the point s lies in the upper half of the complex s plane (Figure 27). We further take

$$\psi_0(r) = U(r) = 0 \text{ for } r > R. \tag{32.6}$$

Then, for $r > R$,

$$\psi(r, s) = f(s)\frac{1}{r}e^{i\sqrt{\frac{2ms}{\hbar}}r} + f_1(s)\frac{1}{r}e^{-i\sqrt{\frac{2ms}{\hbar}}r}. \tag{32.7}$$

For $\sigma > 0$ we define $\sqrt{2ms}$ as the positive root on the positive real axis in the s plane; to ensure single-valuedness, we make a cut along the negative real axis ($\sigma = 0$, $\eta < 0$, $s = \eta + i\sigma$). Clearly, for $\sigma > 0$ the modulus of the first term in (32.7) exponentially decreases for $r \to \infty$ and the modulus of the second term exponentially increases. But for $\sigma > 0$, when $\psi(r, s)$ is defined by a convergent integral, $\psi(r, s)$ is known not to increase for large r. We therefore take $f_1(s) = 0$.

In other words, if $\psi(r, s)$ is defined as the transform of the solution of the time-dependent Sch. Eq. and natural restrictions are imposed on the initial state $\psi_0(r)$, we find that $\psi(r, s)$ should match the outgoing wave

$$\psi(r, s) \xrightarrow[r\to\infty]{} f(s)\frac{1}{r}e^{i\sqrt{\frac{2ms}{\hbar}}r}.$$

This conclusion was originally obtained for the upper s halfplane. As we have already noted, in the lower s halfplane the function $\psi(r, s)$ is defined not by the integral but as the analytic continuation of the $\psi(r, s)$ defined in the upper halfplane. Therefore, the condition of matching with the first term in (32.7) must be retained in the lower halfplane too.

The decaying state satisfies the equation

$$-E\psi_E(r) - \frac{\hbar^2}{2m}\Delta\psi_E(r) + U(r)\psi_E(r) = 0 \tag{32.8}$$

and is matched with an outgoing wave for certain $E = E_0 - i\Gamma/2$. Hence the potential $U(r)$ is such that equation (32.5) with zero right-hand side has a nontrivial solution for $\hbar s = E$.

Hence it follows that the general solution of the inhomogeneous equation (32.5) should have a pole at the point $\hbar s = E$, i.e., in the lower quadrant of the s plane. The solution will have the form

$$\lim_{\hbar s\to E}\psi(r, s) = \frac{a\psi_E(r)}{\hbar s - E} + \psi_1(r, s), \tag{32.9}$$

where $\psi_1(r, s)$ is bounded for $\hbar s = E$.

The problem thus reduces to the determination of the coefficient a. To this end we multiply (32.5) by $\psi_E(r)$ and (32.8) by $\psi(r, s)$, subtract one from the other, and integrate from 0 to R. Remembering that outside the range of the potential for $\hbar s \to E$ we have

$$\psi_E(r) = \frac{C}{r}e^{i\sqrt{\frac{2mE}{\hbar^2}}r}, \quad \psi(r, s) = f(s)\frac{1}{r}e^{i\sqrt{\frac{2ms}{\hbar}}r},$$
$$f(s) = \frac{Ca}{\hbar s - E},$$

we obtain after simple manipulations

$$(\hbar s - E)\left\{\frac{iCf(s)}{\sqrt{\frac{2ms}{\hbar}} + \sqrt{\frac{2mE}{\hbar^2}}} + \right.$$
$$\left. + \int_0^\infty \left[\psi(r, s)\psi_E(r) - f(s)\frac{C}{r^2}e^{\left(i\sqrt{\frac{2ms}{\hbar}} + i\sqrt{\frac{2mE}{\hbar^2}}\right)r}\right] r^2 dr\right\} = \int_0^\infty \psi_0(r)\psi_E(r)r^2 dr.$$

We now insert

$$\psi(r, s) = \frac{a\psi_E(r)}{\hbar s - E} + \psi_1(r, s),$$
$$f(s)\frac{e^{i\sqrt{\frac{2ms}{\hbar}}r}}{r} = \frac{aC}{\hbar s - E}\frac{1}{r}e^{i\sqrt{\frac{2ms}{\hbar}}r},$$

take the limit as $\hbar s \to E$ and extend the integrals to $R = \infty$, remembering that the integrands vanish for $r > R$. All this gives

$$a = \int_0^\infty \psi_0(r)\,\psi_E(r)\,r^2\,dr \Bigg/ \left\{\int_0^\infty \left[\psi_E^2(r) - \left(\frac{Ce^{i\sqrt{\frac{2mE}{\hbar^2}}r}}{r}\right)^2\right] r^2\,dr + \frac{iC^2}{2k}\right\} = \frac{\int_0^\infty (r\psi_0(r))(r\psi_E(r))\,dr}{\int_0^\infty (r\psi_E(r))^2\,dr}, \quad (32.10)$$

where the integral $\int_0^\infty (r\psi_E)^2\,dr = \int_0^\infty \chi_k^2\,dr$ in the denominator is understood in the sense of expression (31.7) of the previous section.

Inserting (32.9) in the inversion formula (32.4), we obtain the contribution from a path bypassing the pole $\hbar s = E$:

$$\psi_t(r,\ t) = a\psi_E(r)\ e^{-\frac{iEt}{\hbar}} = \psi_E(r)\,e^{-\frac{iEt}{\hbar}} \frac{\int_0^\infty (r\psi_0(r))\,(r\psi_E(r))\,dr}{\int_0^\infty (r\psi_E(r))^2\,dr}. \quad (32.11)$$

In this form the expression is entirely analogous to the ordinary expression derived for negative real eigenvalues in a discrete spectrum. The scalar product $\int_0^\infty r^2\psi_0\psi_E dr$ and the norm $\int_0^\infty \psi_E^2 r^2 dr$ in the sense (31.7) enter on equal terms both the perturbation theory and the nonstationary problem.

§ 33. CREATION OF AN UNSTABLE PARTICLE

Suppose that a pair of stable particles react and are converted to a different pair of stable particles:

$$a + X \to b + Y. \quad (33.1)$$

How will the reaction change if one of the product particles, say Y, is unstable and eventually decays, i.e.,

$$Y \to c + d. \quad (33.2)$$

First it is clear that for $r \to \infty$ the particle Y will never be observed; we will only find its decay products. Formally we are thus dealing with a three-particle reaction

$$X + a \to b + c + d. \quad (33.3)$$

In what follows we shall see, however, that this process may follow two distinct courses, or channels

$$X + a \begin{cases} \nearrow\ b + c + d, \\ \searrow\ b + Y \to b + c + d, \end{cases} \quad (33.3')$$

i.e., with direct formation of the three particles and in two stages, when first the reaction produces $b + Y$ and only then does Y decay into $c + d$.

A particle-creating physical process can be described in the following way. The incoming particles collide and form an intermediate state in which the particles are rearranged. The radius R of the intermediate state (reaction radius) is generally of the order of magnitude of the range of the interaction forces between the particles. After a certain time the intermediate state decays either into the original reacting particles or into some other, new particles. The former alternative is the simple case of elastic or inelastic scattering, whereas the latter case is a reaction. The intermediate state can thus be regarded as the source of particles created in the reaction. The particle creation process in reaction (33.1), say, can thus be formally described by a Sch. Eq. with a source:

$$(H_b + H_c + H_d + U_{cd} - E)\varphi = Q, \tag{33.4}$$

where H_b, H_c, H_d are the Hamiltonians of the free particles b, c, and d, U_{cd} is the interaction potential between c and d, and Q is the source function. In general Q depends on the total energy E, but in all the cases that we will deal with this dependence can be neglected.

In equation (33.4) for simplicity we ignored the interaction of particle b with particles c and d. The potential U_{cd}, however, cannot be omitted, since this interaction is directly responsible for the very existence of the unstable particle Y.

We will now derive general expressions for the rates of various reactions described by equation (33.4). To cover the main cases, we will assume the interaction between c and d to be such that

(a) there exists a bound state of the pair $c + d$ with energy $-\varepsilon_0$ ($\varepsilon_0 > 0$); this state we call a particle Y_0;

(b) there exists a quasistationary state of the pair $c + d$ with energy E_0 and width Γ (unstable particle Y).

To facilitate comparison between creation of stable and unstable particles, we assume both Y_0 and Y to have zero spin. Depending on the total energy E, we distinguish between different processes:

1) for $E < -\varepsilon_0$, both reactions are equiprobable from energy standpoint;

2) for $-\varepsilon_0 < E < 0$, only the reaction with formation of Y_0 is possible;

3) if $0 < E < E_0$, in addition to Y, the three particles $b + c + d$ may form in the free state, but the formation of Y is still forbidden;

4) the formation of the particle Y is energetically allowed only for $E > E_0$.

We will now consider the various cases one after the other.

In the center of mass system, the Sch. Eq. has the form

$$\left(-\frac{\hbar^2}{2m}\Delta_\rho - \frac{\hbar^2}{2\mu}\Delta_r + U_{cd}(r) - E\right)\varphi = Q. \tag{33.5}$$

Here r is the distance between c and d,

$$\boldsymbol{r} = \boldsymbol{r}_c - \boldsymbol{r}_d,$$

ρ is the distance from b to the center of mass of the pair $(c+d)$,

$$\boldsymbol{\rho} = \boldsymbol{r}_b - \frac{m_c\boldsymbol{r}_c + m_d\boldsymbol{r}_d}{m_c + m_d},$$

and m and μ are the reduced masses

$$\mu = \frac{m_c m_d}{m_c + m_d}, \quad m = \frac{m_b (m_c + m_d)}{m_b + m_c + m_d}.$$

Using expression (20.2) for Green's function, we write φ in the form

$$\varphi(r, \rho) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\varepsilon\, G_{\varepsilon}^{(+)}(r, r_1)\, G_{E-\varepsilon}^{(+)}(\rho, \rho_1)\, Q(r_1, \rho_1)\, dr_1\, d\rho_1, \tag{33.6}$$

where G_ε and $G_{E-\varepsilon}$ are the one-particle Green's functions

$$\left(-\frac{\hbar^2}{2\mu}\Delta_r + U_{cd} - \varepsilon\right) G_{\varepsilon}^{(+)}(r, r_1) = \delta(r - r_1),$$
$$\left(-\frac{\hbar^2}{2m}\Delta_\rho - (E - \varepsilon)\right) G_{E-\varepsilon}^{(+)}(\rho, \rho_1) = \delta(\rho - \rho_1).$$

The wave function $\varphi(r, \rho)$ depends on two coordinates. However, it is clear that to find the number of creation events of the three free particles $b + c + d$ it is sufficient to find the current of one particle only, say b. We thus expand $\varphi(r, \rho)$ in eigenstates of the pair $c + d$.

The complete system of wave functions of the pair $c + d$ comprises the wave function of the bound state (the particle Y_0) $\frac{1}{\sqrt{4\pi}} \frac{1}{r} \chi_0(r)$ and the continuum wave functions $\psi_k^{(+)}(r)$ normalized to $\delta(k - k_1)$. The expansion thus has the form

$$\varphi(r, \rho) = \Phi_0(\rho) \frac{1}{\sqrt{4\pi}} \frac{\chi_0(r)}{r} + \int dk\, \psi_k^{(+)}(r)\, \Phi_k(\rho), \tag{33.7}$$

where

$$\left.\begin{aligned} \Phi_0(\rho) &= \int \varphi(r, \rho) \frac{1}{\sqrt{4\pi}} \frac{1}{r} \chi_0^*(r) dr, \\ \Phi_k(\rho) &= \int \varphi(r, \rho)\, \psi_k^{(+)*}(r) dr. \end{aligned}\right\} \tag{33.7'}$$

The left-hand sides of these expressions can be treated as wave functions of particle b when the pair $c + d$ is formed in the bound state and in the continuum state, respectively.

Using the properties of Green's functions from Chapter 4 and the relation

$$\frac{1}{2\pi i} \int_{-\infty}^{\infty} d\varepsilon_1\, G_{E-\varepsilon_1}^{(+)}(\rho, \rho_1) \frac{1}{\varepsilon_1 - \varepsilon + i\gamma} = -G_{E-\varepsilon}(\rho, \rho_1),$$

we find from (33.6)–(33.7')

$$\left.\begin{aligned} \Phi_0(\rho) &\underset{\rho\to\infty}{\sim} \frac{e^{iq_0\rho}}{\rho} \frac{2m}{\hbar^2} \frac{1}{4\pi} \int dr_1\, d\rho_1 Q(r_1, \rho_1)\, e^{iq_0 \frac{\rho\rho_1}{\rho}} \frac{1}{\sqrt{4\pi}} \frac{\chi_0^*(r_1)}{r_1} \equiv \frac{e^{iq_0\rho}}{\rho} f_0, \\ \Phi_k(\rho) &\underset{\rho\to\infty}{\sim} \frac{e^{iq\rho}}{\rho} \frac{2m}{\hbar^2} \frac{1}{4\pi} \int dr_1\, d\rho_1 Q(r_1, \rho_1)\, e^{iq \frac{\rho\rho_1}{\rho}}\, \psi_k^{(+)*}(r_1) \equiv \frac{e^{iq\rho}}{\rho} f_k. \end{aligned}\right\} \tag{33.8}$$

Here

$$q_0 = \sqrt{\frac{2m}{\hbar^2}(E + \varepsilon_0)}, \quad q = \sqrt{\frac{2m}{\hbar^2}(E - \varepsilon)}, \quad \varepsilon = \frac{\hbar^2 k^2}{2\mu};$$

the asymptotic expressions for $\rho \to \infty$ were obtained using (18.13).

In general the amplitudes f_0 and f_k depend not only on E and ε but also on the direction of the vector $\boldsymbol{\rho}$. The radius R of the source is assumed to be sufficiently small so that $qR \ll 1$. The exponential function in the integrand may thus be replaced by unity and the dependence on $\frac{\boldsymbol{\rho}}{\rho}$ drops out. The functions Φ thus become spherically symmetric. Physically this corresponds to a case when the product particle b is formed in the s-state only.

The total yield of the reaction producing the particle b and the bound state Y_0 of the pair $c + d$ is equal to the current integrated over the surface of a large sphere:

$$j_{Y_0} = \int \rho^2 \, d\Omega_\rho \frac{i\hbar}{2m} (\Phi_0 \nabla_\rho \Phi_0^* - \Phi_0^* \nabla_\rho \Phi_0) = 4\pi v_{q_0} |f_0|^2, \; v_{q_0} = \frac{\hbar q_0}{m}.$$

$d\Omega_\rho$ is the solid angle element in the direction of the vector $\boldsymbol{\rho}$.

Similarly the yield $j(\boldsymbol{k})\, d\boldsymbol{k}$ of the reaction in which the momentum of relative motion of the particles $c + d$ lies in the interval $d\boldsymbol{k}$ around $\boldsymbol{k}$ is given by

$$j(\boldsymbol{k})\, d\boldsymbol{k} = 4\pi v_q |f_k|^2 \, d\boldsymbol{k}, \; v_q = \frac{\hbar q}{m}.$$

Integrating over all the directions of the vector $\boldsymbol{k}$ and changing from $d\boldsymbol{k}$ to $d\varepsilon$, we find

$$\begin{gathered} j(\varepsilon)\, d\varepsilon = \sum_{lm} j_{lm}(\varepsilon)\, d\varepsilon, \\ j_{lm}(\varepsilon) = \frac{4\pi}{\hbar} \frac{v_q}{v} \left| \int dr_1 \, d\rho_1 Y_{lm}\left(\frac{r_1}{r_1}\right) \frac{1}{r_1} \chi_{lm}(r_1)\, Q(r_1, \rho_1) \frac{2m}{\hbar^2} \frac{1}{4\pi} \right|^2. \end{gathered} \tag{33.9}$$

Here $j_{lm}(\varepsilon)$ is the reaction yield for a given energy ε and given quantum numbers l, m of the relative motion of particles $c + d$.

Let us compare the yields of two-particle and three-particle reactions. To estimate j_{Y_0} note that the radius of Y_0 is of the order $\frac{1}{k_0} \equiv \left(\frac{\hbar^2}{2\mu\varepsilon_0}\right)^{1/2}$, so that the radial function $\chi_0(r)$ normalized to unity is of the order of $\left(\frac{2\mu\varepsilon_0}{\hbar^2}\right)^{1/4}$. The total reaction yield for Y_0 is

$$\begin{gathered} j_{Y_0} = A_0 \sqrt{\varepsilon_0 (E + \varepsilon_0)}; \\ A_0 = 2 \sqrt{\frac{\mu}{m}} \frac{1}{\hbar} \left| \frac{2m}{\hbar^2} \frac{1}{4\pi} \int dr_1 \, d\rho_1 \frac{Q(r_1, \rho_1)}{r_1} \right|^2. \end{gathered} \tag{33.10}$$

Here A_0 is independent of energy.

Now consider the yield of the three-particle reaction $X + a \to b + c + d$. The total energy E is first assumed to be less than the energy E_0 of the quasistationary pair $c + d$ (the particle Y), so that the formation of the latter is forbidden by energy considerations. All the three particles b, c, d are thus emitted from the source Q independently.

At low energies the entire yield is determined only by the term $j_{00}(\varepsilon)\, d\varepsilon$ in (33.9). This is so because $\chi_{kl}(r_1) \sim (kr_1)^{l+1}$ and for $l > 0$ the corresponding terms give a negligible contribution. To estimate $j_{00}(\varepsilon)\, d\varepsilon$ note that $\chi_{k0}(r_1)$ in the integrand in (33.9) can be approximately replaced by kR (where R is the radius of the source Q). We thus get

$$j(\varepsilon)\, d\varepsilon = A_0 \sqrt{\varepsilon (E - \varepsilon)} \frac{d\varepsilon}{2\varepsilon_1}; \; \varepsilon_1 = \frac{\hbar^2}{2\mu R^2}. \tag{33.11}$$

Here A_0 is the same constant as in (33.10), and ε_1 is a constant having the dimension of energy. Numerically it is equal to the energy of a particle of mass μ confined within a volume of radius R. In nuclear physics $\varepsilon_1 \sim 1$ MeV and in elementary particle physics $\varepsilon_1 \sim 100$ MeV.

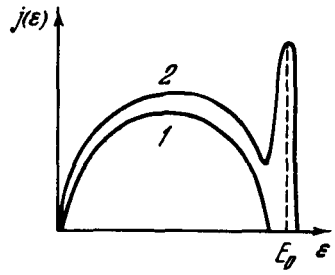

FIGURE 28.

The energy distribution of particles in a three-particle reaction is given by (33.11). The function $j(\varepsilon)$ is plotted by curve 1 in Figure 28. The total yield of a three-particle reaction is

$$j = \int_0^E j(\varepsilon)\, d\varepsilon = A_0 \frac{\pi}{16\varepsilon_1} E^3. \tag{33.11}$$

We now increase the energy E until it becomes comparable with E_0 and the formation of the unstable particle Y becomes possible. Let us consider $j_{00}(\varepsilon)$ for $\varepsilon \approx E_0$. The radial wave function $\chi_{k_\varepsilon}(r)$ near the resonance is highly sensitive to energy and may reach high values. The corresponding expressions were derived in the preceding (see (27.6) and (27.7)). Inserting them in (33.9) we obtain

$$j_{00}(\varepsilon)\, d\varepsilon = A_0 \frac{2}{\pi} \left(\frac{\varepsilon_1}{E_0}\right)^{1/4} \frac{2E_0}{\Gamma} \frac{\Gamma^2/4}{(\varepsilon - E_0)^2 + \Gamma^2/4} \frac{\sqrt{\varepsilon(E-\varepsilon)}}{2\varepsilon_1} d\varepsilon. \tag{33.12}$$

We see that $j_{00}(\varepsilon)$ has a sharp maximum for $\varepsilon \approx E_0$ (curve 2 in Figure 28). The resonance factor is responsible for the marked increase of the reaction yield at $\varepsilon \approx E_0$. The physical reason for this is fairly obvious: at $\varepsilon \approx E_0$ the product is a single quasistationary particle Y, and not two independent particles c and d, so that we are in fact dealing with a two-particle reaction.

The width $\Delta\varepsilon$ around $\varepsilon = E_0$ where the two-particle reaction is dominant is determined from the condition (we take for simplicity $\varepsilon_1 \approx E_0$)

$$\frac{2E_0}{\Gamma} \frac{\Gamma^2/4}{(\Delta\varepsilon)^2 + \Gamma^2/4} = 1, \text{ i.e., } \Delta\varepsilon = \sqrt{\frac{E_0\Gamma}{2}} = \sqrt{\frac{E_0}{2\Gamma}}\,\Gamma.$$

Let us calculate the total yield j_Y of particles Y at energy E close to E_0. To this end we integrate (33.12) over ε in the "two-particle" region $E_0 - \Delta\varepsilon \leqslant \varepsilon \leqslant E$:

$$j_Y = \int_{E_0-\Delta\varepsilon}^{E} d\varepsilon j_{00}(\varepsilon) \approx A_0 \sqrt{\varepsilon_1}\, \mathrm{Re}\left[E - \left(E_0 - \frac{i\Gamma}{2}\right)\right]^{1/2}. \tag{33.13}$$

The energy dependence of the yield is determined by a factor first derived in /184/

$$\mathrm{Re}\left[E-\left(E_0-\frac{i\Gamma}{2}\right)\right]^{1/2}=\frac{1}{\sqrt{2}}\left[\sqrt{(E-E_0)^2+\frac{\Gamma^2}{4}}+(E-E_0)\right]^{1/2}\approx$$

$$\approx\begin{cases}(E-E_0)^{1/2}\left[1+\left(\dfrac{\Gamma}{4(E-E_0)}\right)^2+\cdots\right] & \text{for } E\gg E_0+\dfrac{\Gamma}{2},\\ \dfrac{\Gamma}{4(E_0-E)^{1/2}} & \text{for } E\ll E_0-\dfrac{\Gamma}{2}.\end{cases}$$

The graph of this curve is shown in Figure 29.

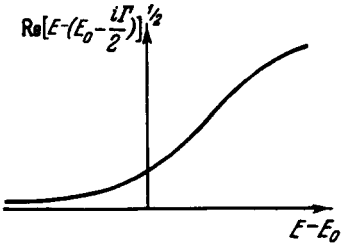

FIGURE 29.

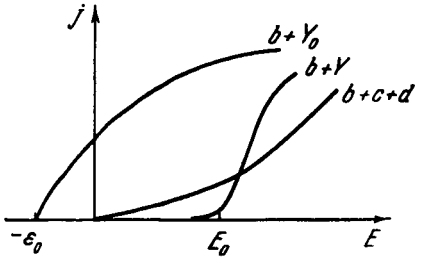

FIGURE 30.

We thus have the following picture. Starting with $E=-\varepsilon_0$, a stable particle Y_0 may form. The reaction yield $b+Y_0$ is specified by (33.10). The yield as a function of energy is shown in Figure 30. Starting with $E=0$, the three-particle reaction is turned on (see (33.11)). For low E the three-particle yield is very insignificant ($\sim E^2$). Finally for $E\gtrsim E_0$ the formation of the unstable particle Y begins.

§ 34. TRANSITION FROM QUASISTATIONARY TO STATIONARY STATES

It is highly significant that the energy dependence of the yield of the unstable particle Y turned to be very close to the energy dependence of the pure two-particle reaction with Y_0 as one of the end products. For $\Gamma\to 0$ the likeness is virtually complete. Another significant point is that the absolute yields are also fairly close to one another. To eliminate the effect of kinetic factors (the final state phase volume), the yields should be compared at equal distances from the respective thresholds. In this case we have

$$\frac{\text{yield }(b+Y)}{\text{yield }(b+Y_0)}=\sqrt{\frac{\varepsilon_1}{\varepsilon_0}}\sim 1.$$

The analogy between quasistationary and stationary states is very considerable, although at a first glance they are fundamentally different: stationary states have a discrete spectrum, whereas the quasistationary states lie in the continuum; the wave functions of the stationary states are localized in a certain region in space, whereas those of quasistationary

states are "spread" over the entire space. In the limit as $\Gamma \to 0$, however, a quasistationary state should go over to a stationary one. Physically this is obvious. We will now try to go into the formal side of the matter.

The most characteristic feature of wave functions describing quasistationary states is that they have an exceptionally high magnitude inside the potential range (this has been discussed before, see (27.7)):

$$\int_0^R \chi_k^2(r)\,dr = \frac{\hbar}{\pi}\frac{v_0\Gamma/2}{(E-E_0)^2+\Gamma^2/4}. \tag{34.1}$$

For example, for radium $R \sim 10^{-12}$ cm, decay energy $E_0 \sim 10$ MeV $\approx 10^{-5}$ erg, lifetime $T_{1/2} \approx 5000$ years (i.e., $\Gamma \sim 10^{-38}$ erg). For $E = E_0$ this formula gives

$$\int_0^R \chi_k^2\,dr \approx 10^{19}\ \text{cm}.$$

To give a rough idea of the staggering value of this integral, it suffices to mention that in the integral of the square of the modulus of the α-particle wave function over a volume with a radius of 10 light years

$$\int_0^{10\ \text{light years}} \chi_k^2\,dr$$

the dominant contribution is from the central core $r \leqslant 10^{-12}$ cm. It is only when integrating over a sphere with a radius greater than 10^{15} km ~ 100 light years that the "outer" part of the wave function having the form $\sqrt{\frac{2}{\pi}}\sin(kr+\delta)$ starts making a noticeable contribution.

Since any integral used in practice (even if formally taken between infinite limits) implies integration inside a much smaller radius (of the order of interatomic distances, say), it is clear that the wave function "tails" extending to infinity are ignorable. In this sense, the wave function of the radium nucleus is actually localized within a volume of 10^{-12} cm radius, although formally it is a continuum function and "fills" the entire space.

Another manifestation of the large value of χ_k in the resonance region (or, equivalently, of the long lifetime of the quasistationary state) is the form of the energy spectrum of the particles $b + c + d$ for $E > E_0$. Formally $c + d$ may have any energy between $0 < \varepsilon < E$, but in practice, as we have seen in the previous section (see Figure 28), a considerable fraction of particles are created almost with the exact energy of relative motion $\varepsilon = E_0$.

The analogy between quasistationary and stationary states can be formulated in more exact terms.

Consider a function $f(r)$ which increases sufficiently fast with increasing r. We expand it in eigenfunctions $\chi_k(r)$ of the Sch. Eq. with a potential which has a quasistationary level (see Figure 18) at $k = k_0$.

The expansion coefficients $C(k)$ are given by

$$C(k) = \int_0^\infty f(r')\,\chi_k(r')\,dr'. \tag{34.2}$$

The contribution from the interval $0 < k < \varkappa_0$ to this expansion is

$$\int_0^{\varkappa_0} C(k)\,\chi_k(r)\,dk = \int_0^{\varkappa_0} \chi_k(r) \int_0^{\infty} \chi_k(r_1) f(r_1)\,dr_1\,dk. \tag{34.3}$$

The main contribution to this integral comes from the region $k \approx k_0$ and $r < R$. In this region we may write (see § 27)

$$\chi_k(r) \approx A(k)\,\chi_k^{(0)}(r), \tag{34.4}$$

where $\chi_k^{(0)}$ is not very sensitive to energy. Therefore (34.3) can be written in the form

$$\chi^{(0)}(r) \int_0^{\varkappa_0} A^2(k)\,dk \int_0^{\infty} f(r_1)\,\chi^{(0)}(r_1)\,dr_1 = \chi^{(0)}(r) \int_0^{\infty} \chi^{(0)}(r_1) f(r_1)\,dr_1, \tag{34.5}$$

where we used the explicit expression for $A(k)$:*

$$\int_0^{\varkappa_0} A^2(k)\,dk \approx \int_{-\infty}^{\infty} \frac{k_0}{\pi} \frac{(\Gamma/2)\,dk}{(E-E_0)^2+\Gamma^2/4} = \frac{1}{\pi}\int \frac{(\Gamma/2)\,dE}{(E-E_0)^2+\Gamma^2/4} = 1. \tag{34.6}$$

Since $A^2(k)$ has a sharp maximum at $E = E_0$, we approximately have from (34.6)

$$A^2(k) = \delta(k - k_0).$$

In this approximation the expansion of any function

$$f(r) = \int_0^{\infty} C(k)\,\chi_k(r)\,dk = \chi^{(0)}(r) \int_0^{\infty} \chi^{(0)} f\,dr_1 + \int_{\varkappa_0}^{\infty} C(k)\,\chi_k\,dk \tag{34.7}$$

has a form which as if corresponds to a continuous spectrum beginning only at $k = \varkappa_0$, whereas in the interval $0 \leqslant k \leqslant \varkappa_0$ there is a single stationary state $\chi^{(0)}(r)$. (This is an obvious idealization associated with the approximate character of the formula (34.4), but the corrections become smaller as Γ decreases and as the range of the function $f(r)$ shrinks.)

The fact that in various expansions of the form (34.7) quasistationary and stationary states are entirely equivalent is the formal reason for the great similarity of these two kinds of states.

§ 35. COLLISION TIME

The treatment of lifetime of quasistationary states has so far been largely intuitive. We will now go into this question more rigorously. Consider the following problem /185/: a particle of given energy E is scattered by a potential V of range R. What is the mean time $T(E, a)$ that the particle spends inside a sphere of radius $r = a$, $a \geqslant R$?

* As is usual, the function $\chi_k^{(0)}$ is normalized by the condition

$$\int_0^R |\chi_k^{(0)}|^2\,dr = 1.$$

We have to devise a mechanism which would function as a clock ticking off the time that the particle spends inside a sphere of radius $r = a$. The following "clock" mechanism can be proposed: suppose that inside the sphere $r = a$ there is a weak homogeneous magnetic field H directed along the z axis, which is zero for $r > a$, and let the incident particles have a magnetic moment μ. Let further, the incoming particles be polarized along the x axis (so that their magnetic moments are aligned along the x axis). As long as a particle stays outside the sphere $r = a$, there are no forces acting on the magnetic moment and its direction does not change. However, as soon as the particle enters the sphere $r \leqslant a$, where a magnetic field is present, the magnetic moment will start precessing about the field vector with a frequency $\omega = \frac{2\mu H}{\hbar}$. (The change of particle energy due to the interaction $-\mu H$ is negligible for small H.) The precession will go on as long as the particle remains inside the sphere $r = a$. If the time that the particle spends inside the sphere is T, the magnetic moment will have rotated through an angle $\theta = T\omega$ in the xy plane by the time the particle emerges from the sphere. Thus, given the precession angle of the magnetic moment of the scattered particles, we can readily compute the mean time that the particle spends inside the sphere $r = a$. The results give

$$T(E, a) = \frac{2}{v}\left\{\frac{d\delta}{dk} + a - \frac{1}{2k}\sin 2(ka + \delta)\right\}. \tag{35.1}$$

To derive this expression, let us calculate the precession angle θ of the magnetic moment.

When a magnetic field is turned on, the Sch. Eq. takes the form (for simplicity we only consider the case $l = 0$ case)

$$\hat{\chi}'' + (k^2 - V)\hat{\chi} = -\frac{2m}{\hbar^2}\mu H\hat{\chi} = -\frac{2m}{\hbar^2}\mu H\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\hat{\chi}. \tag{35.2}$$

The term in the right-hand side describes the interaction $-\mu H$; since by assumption the vector H is directed along the z axis and μ inevitably has the form $\mu = 2\mu s$, where s is the particle spin vector,* taken equal to $1/2$, we have

$$\mu H = 2\mu s_z H = \mu\sigma_z H = \mu H\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix},$$

where σ_z is the Pauli matrix. Since the particle spin $s = 1/2$, the wave function $\hat{\chi}$ is to be understood as the column

$$\hat{\chi} = \begin{pmatrix}\chi_1\\ \chi_2\end{pmatrix},$$

where χ_1 and χ_2 describe the two states with respective spin projections of $+1/2$ and $-1/2$ on the z axis.

* The spin vector s is the only pseudovector characterizing a particle at rest. The pseudovector μ must therefore be proportional to s.

The problem is solved by perturbation theory. The zeroth-approximation wave function $\hat{\chi}^{(0)}$ by assumption describes a state with μ directed along the x axis. This function is

$$\hat{\chi}^{(0)} = \chi_k(r)\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix},$$

where $\chi_k(r)$ is the solution of the homogeneous equation (35.2), which has the asymptotic form

$$\chi_k(r) \sim \sqrt{\frac{2}{\pi}}\sin(kr+\delta).$$

The solution of equation (35.2) is sought in the form

$$\hat{\chi} = \hat{\chi}^{(0)} + \hat{\chi}^{(1)} \equiv \hat{\chi}^{(0)} + \begin{pmatrix}\chi_1^{(1)}\\ \chi_2^{(1)}\end{pmatrix}.$$

To first approximation we have

$$(\hat{\chi}^{(1)})'' + (k^2 - V)\hat{\chi}^{(1)} = -\frac{2m}{\hbar^2}\mu H\hat{\chi}^{(0)}.$$

Writing separate equations for the two components, we obtain

$$(\chi_1^{(1)})'' + (k^2 - V)\chi_1^{(1)} = -\frac{2m}{\hbar^2}\mu H\frac{1}{\sqrt{2}}\chi_k(r),$$
$$\chi_2^{(1)''} + (k^2 - V)\chi_2^{(1)} = \frac{2m}{\hbar^2}\mu H\frac{1}{\sqrt{2}}\chi_k(r).$$

Using Green's function, we write the solution in the form

$$\chi_1^{(1)} = -\chi_2^{(1)} = -\frac{2m}{\hbar^2}\mu H\frac{1}{\sqrt{2}}\int G_k(r, r_1)\chi_k(r_1)\,dr_1 \sim$$
$$\sim \frac{2m}{\hbar^2}\mu H\frac{1}{\sqrt{2}}\sqrt{\frac{\pi}{2}}\frac{1}{k}e^{i(kr+\delta)}\int_0^a \chi_k^2(r_1)\,dr_1 \equiv$$
$$\equiv \frac{\beta}{2\sqrt{\pi}}e^{i(kr+\delta)},\quad \beta = \frac{2m}{\hbar^2}\mu H\frac{\pi}{k}\int_0^a \chi_k^2(r_1)\,dr_1.$$

Collecting all the formulas, we obtain the following asymptotic expression for the solution of equation (35.2):

$$\hat{\chi} = \hat{\chi}^{(0)} + \hat{\chi}^{(1)} \sim \frac{i}{\sqrt{2\pi}}\left\{\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}e^{-i(kr+\delta)} - \frac{1}{\sqrt{2}}\begin{pmatrix}1+i\beta\\1-i\beta\end{pmatrix}e^{i(kr+\delta)}\right\}. \qquad (35.3)$$

The first term in braces describes the incident particles and the second term describes the scattered particles.

Let us calculate the spin precession angle θ. The mean values of the spin x and y components are (in calculations we ignore terms $\sim\beta^2 \sim H^2$)

$$\bar{s}_x = \frac{1}{\sqrt{2}}\begin{pmatrix}1+i\beta\\1-i\beta\end{pmatrix}^+\frac{1}{2}\begin{pmatrix}0&1\\1&0\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}1+i\beta\\1-i\beta\end{pmatrix} = \frac{1}{2},$$
$$\bar{s}_y = \frac{1}{\sqrt{2}}\begin{pmatrix}1+i\beta\\1-i\beta\end{pmatrix}^+\frac{1}{2}\begin{pmatrix}0&-i\\i&0\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}1+i\beta\\1-i\beta\end{pmatrix} = -\beta.$$

The absolute value of the precession angle is thus $\theta = 2\beta$ and for the lifetime we easily find by (15.18)

$$T(E, a) = \frac{\theta}{\omega} = \frac{2\beta\hbar}{2\mu H} = \frac{2}{v}\left\{\frac{d\delta}{dk} + a - \frac{1}{2k}\sin 2(ka + \delta)\right\},$$

which was to be proved.

Let us now return to quasistationary states. Inserting expression (27.4) for the phase in (35.1) and dropping all terms apart from the leading term, we obtain

$$T(E) = \frac{\hbar\Gamma}{(E - E_0)^2 + \Gamma^2/4}. \tag{35.4}$$

This result confirms our previous conclusion concerning the mean lifetime of a quasistationary state and the dependence of this lifetime on the exact particle energy.

Expression (35.1), as we see from its derivation, corresponds to the a v e r a g e time $\bar{T}$ that the particle spends inside the sphere $r = a$. It would therefore seem that the actual time T that the particle spends in the region $r \leqslant a$ is not a deterministic quantity, and there is in fact a certain distribution of these times $W(T)$.

It is readily seen, however /186/, that this distribution has the form of a δ-function, $W(T) \sim \delta(T - \bar{T})$. The time T is thus a fixed quantity for a given energy E!

Note that this in no way clashes with the uncertainty relation $\Delta E \cdot \Delta t \geqslant \hbar$. Indeed, examining the motion of wave packets, we readily conclude that the Δt here is the uncertainty at the exact collision instant. It has no relation whatsoever to the d u r a t i o n of collision.

§ 36. OTHER TYPES OF LONG-LIVED STATES

It would be wrong to suppose that the resonance states dealt with in this chapter constitute the only type of relatively long-lived states of a particle which lie in the continuum. There are at least two other types of states ("virtual level" and "threshold state") whose lifetimes may considerably exceed the characteristic time of flight /187/.

Before we can proceed with a discussion of these states, consider the case of a free particle moving with orbital momentum $l = 0$ relative to the origin. According to the general expression (35.1) such a particle remains inside a sphere of radius R during the time

$$T_{\text{fr}} = \frac{2}{v}\left\{R - \frac{1}{2k}\sin 2kR\right\}. \tag{36.1}$$

If $kR \gg 1$, i.e., $\lambda \ll R$, where λ is the particle wavelength, the second term in braces can be dropped in comparison with the first term, and we obtain the classical result

$$T_{\text{fr}} = T_{\text{cl}} = \frac{2R}{v}.$$

The time T is equal to the time of flight of the particle through the sphere, and the trajectory passes through the center of the sphere.

The situation radically changes if $kR \lesssim 1$. In this case the wavelength λ is comparable with or greater than the sphere radius. According to quantum mechanics, a particle may have $l = 0$ without actually passing through the point $r = 0$: it is sufficient that the particle be at a distance of the order λ from the origin. Therefore the time the particle spends inside the sphere $r = R$ should be less than the classical time of flight T_{cl}. Indeed, by (36.1) we have for $kR \ll 1$

$$T_{ft} = \frac{4}{3v} k^3 R^3 \underset{k \to 0}{\to} 0. \tag{36.1'}$$

Now suppose that a particle moves in a potential field with a virtual level (or a real level) with low binding energy. In this case the expressions of § 3 are applicable and the scattering phase δ is obtained from the equation

$$k \cot \delta = -\frac{1}{a}, \tag{36.2}$$

where the constant a is the scattering length. For $a < 0$ there is a virtual level with energy $\frac{\hbar^2}{2ma^2}$, and for $a > 0$ a real level with binding energy $\frac{\hbar^2}{2ma^2}$. Solving (36.2) for the phase δ and inserting the result in the expression for lifetime (35.1), we obtain for small kR ($|a| \gg R$)

$$T_{virt} = \frac{2R}{v} \frac{2a^2k^2}{1 + a^4k^2}.$$

The dependence of T on particle energy (or more precisely on k) is shown in Figure 31. We see that the lifetime T_{virt} has a peak at $k \sim \frac{1}{|a|}$, and near this maximum it is greater than the classical time of flight. This is the result of the attractive action of the potential. The attractive effect is particularly pronounced if we compare T_{virt} with the time T_{ft}, (36.1'), that a free particle remains inside the sphere $r = R$. The time ratio

$$\frac{T_{virt}}{T_{ft}} = 3\left(\frac{a}{R}\right)^3 \frac{1}{1 + (ka)^2}$$

may reach very high values for $k \to 0$. Taking $R = 2.5 \cdot 10^{-13}$ cm, we obtain for the triplet neutron-proton interaction ($a \approx 5.4 \cdot 10^{-13}$ cm) a time ratio of ≈ 12; for the singlet interaction ($a = -20 \cdot 10^{-13}$ cm) this ratio is even higher (≈ 200).

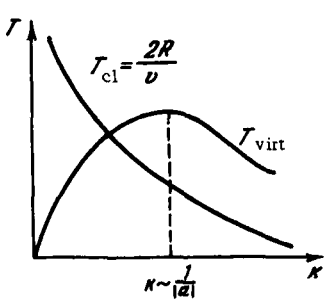

FIGURE 31.

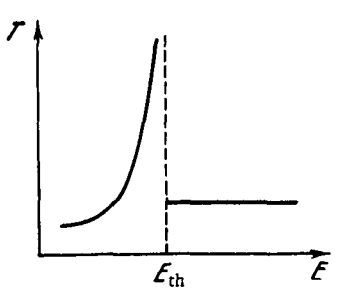

FIGURE 32.

A "virtual level" is thus not simply a convenient mathematical fiction but a real physical state of the system in which the particle spends a considerable length of time inside the potential.

There is another extensive class of relatively long-lived states ("threshold states"). In Chapter 7 we will show that in case of a reaction

$$X + a \to b + Y, \tag{36.3}$$

the phase δ of the elastic scattering ($X + a \to X + a$) on approaching the reaction threshold from below behaves as

$$\delta \approx \delta_0 + \alpha \sqrt{E_{\text{th}} - E},$$

where δ_0 and α are some constants and E_{th} is the threshold energy. The phase derivative $\frac{d\delta}{dk}$ goes to infinity as E approaches E_{th}. The lifetime therefore steadily increases on approaching the threshold point from below (Figure 32).

In principle other kinds of long-lived states are possible, such as states corresponding to multiple poles of the S-matrix /188—190/.

Chapter 6

FUNDAMENTAL PROPERTIES OF MULTICHANNEL SYSTEMS

§ 37. THE WAVE FUNCTION OF A MULTICHANNEL SYSTEM

We have so far dealt with particles in a potential field. The only physical process that can be identified with this idealized situation is elastic scattering. As we know, any collision problem involving two particles with an interaction describable by a potential $U(r_1 - r_2)$ can be reduced to the scattering of a particle off a potential.

Besides the simple case of scattering, we often have to deal with reactions, which convert incoming particles into different particles. Consider for example the following situation. We start with N pairs of particles $a_i + X_i$ $(i = 1, 2, \ldots, N)$ which can transform into one another (whenever this transformation does not clash with energy conservation):

$$a_i + X_i \rightleftarrows a_j + X_j. \tag{37.1}$$

The total mass of each pair will be denoted $M_i = m_{a_i} + m_{X_i}$ and let $M_1 < M_2 < \ldots < M_N$. In all the cases of physical relevance the interaction between particles is represented by short-range forces, i.e., it is ignorable for $r > R$, where R is the interaction range. Thus, in what follows, reactions (37.1) are assumed to be confined inside the sphere $r < R$. We thus arrive at the following picture. In the outer region $(r > R)$, the most general wave function of the system should have the form

$$\Psi = \sum_i (\alpha_i \psi_i^{(-)} - \beta_i \psi_i^{(+)}) \Phi_i; \quad \Phi_i = \Phi(a_i) \Phi(X_i), \tag{37.2}$$

where $\Phi(a_i)$ and $\Phi(X_i)$ are the interior wave functions of particles a_i and X_i (in general, these may be compound particles), α_i and β_i are some constants, $\psi_i^{(-)}$ and $\psi_i^{(+)}$ are two independent solutions of the Sch. Eq. for the pair $a_i + X_i$ in the outer region $r > R$ (we have assumed that the transitions between particles are possible only in the interior region; in the outer region, a_i and X_i are coupled only by long-range Coulombic or centrifugal potentials and the particle motion is thus described by the usual Sch. Eq.) For simplicity, we consider spinless particles and only states with

definite l. The wave functions $\psi_i^{(\pm)}$ are henceforth normalized by the following conditions (only the radial part is considered):

$$\left.\begin{aligned} \psi_{i\,r_i\to\infty}^{(\pm)} &\sim \frac{1}{\sqrt{v_i}}\frac{1}{r_i}e^{\pm i\left(k_i r_i - \frac{l\pi}{2}\right)} && \text{uncharged particles,}\\ \psi_{i\,r_i\to\infty}^{(\pm)} &\sim \frac{1}{\sqrt{v_i}}\frac{1}{r_i}e^{\pm i\left(k_i r_i - \frac{l\pi}{2} + \eta_l + \alpha \ln 2k_i r_i\right)} && \text{charged particles.}\end{aligned}\right\} \qquad (37.3)$$

Here v_i is the relative velocity, k_i is the wave vector, r_i is the distance between a_i and X_i. This normalization corresponds to unit current through the surface of a large sphere.

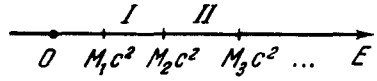

FIGURE 33.

What is the form of the wave function for various energies? To answer this question, we start with the physical requirement of bounded ψ. Consider the energy range $M_3c^2 > E > M_1c^2$ (I in Figure 33). If M_1c^2 is adopted as the zero point of the energy scale, then writing $Q_i = (M_i - M_1)c^2$ for the difference in the rest energies of the 1st and the i-th pair, we obtain for the wave vector of the i-th pair in (37.3)

$$k_i = \sqrt{\frac{(E - Q_i)2\mu_i}{\hbar^2}},\quad \mu_i = \frac{m_{a_i} m_{X_i}}{M_i}. \qquad (37.4)$$

In interval I ($E < Q_2$), all k_j are imaginary, $k_j = i\,|k_j|$, except k_1 which is real. Therefore all the functions $\psi_j^{(-)}$ with $j > 1$ increase exponentially at infinity, $\psi_j^{(+)}$ ($j > 1$) fall off exponentially, and $\psi_1^{(\pm)}$ are everywhere bounded for $r > R$.

The boundedness condition at infinity can thus be satisfied only if we take

$$\alpha_i = 0 \quad (i > 1). \qquad (37.5)$$

In this case Ψ for $r > R$ should have the form

$$\Psi = (\alpha_1\psi_1^{(-)} - \beta_1\psi_1^{(+)})\,\Phi_1 - \sum_{i=2}^{N}\beta_i\psi_i^{(+)}\Phi_i, \qquad (37.6)$$

i.e., it contains an incoming and an outgoing wave of the pair $a_1 + X_1$ (the first term) and a sum Σ which describes the exponentially decaying functions of the other channels. Physically it corresponds to the following case: for $E < Q_2$, a_1 and X_1 are the only particles which may escape to infinity, whereas all the other pairs $a_i + X_i$ ($i > 1$) cannot exist in the free state since the energy is insufficient; they are only virtually created in the interior region and slightly "stick out" into the exterior region (this is described by the decaying "tails" in the second term in (37.6)).

The only physical process which may occur at energies $E < Q_2$ is thus elastic scattering of the particles a_1 and X_1. In any theory the wave function of elastic scattering should be completely determinable by the amplitude of the incident wave, in our case the coefficient α_1. Dividing (37.6) by α_1, we write this result in the form

$$\Psi_1 = \psi_1^{(-)}\Phi_1 - \sum_{i=1}^{N} S_{i1}\psi_i^{(+)}\Phi_i. \qquad (37.7)$$

Here $S_{i1} \equiv \frac{\beta_i}{\alpha_i}$ are entirely determined by the Hamiltonian of our multichannel system. They are naturally functions of energy. We can find them only if the wave function in the interior region is known; matching the wave function and its derivative at $r = R$ with (37.7), we obtain an equation for S_{i1}.

By the law of conservation of the number of particles, the amplitudes of the incident and the outgoing wave should be equal. This directly leads to the familiar equality

$$|S_{11}| = 1 \text{ for } 0 < E < Q_2.$$

The other coefficients S_{i1} are quite arbitrary between certain limits /191/.

We now increase the energy so that $Q_2 < E < Q_3$ (II in Figure 33). In this range, $\psi_i^{(-)}$ with $i > 2$ is divergent at infinity, whereas the functions $\psi_1^{(\pm)}$, $\psi_2^{(\pm)}$, and $\psi_{i>2}^{(+)}$ are bounded everywhere for $r > R$. Therefore the boundedness condition for the wave function at infinity now leads to the condition

$$\alpha_i = 0 \text{ for } i > 2. \tag{37.8}$$

The amplitudes of the incoming waves of the first two channels α_1 and α_2 can be selected quite arbitrarily. One independent solution is obtained by taking, say, $\alpha_1 = 1, \alpha_2 = 0$. The second solution can be defined by $\alpha_1 = 0$, $\alpha_2 = 1$. The physical meaning of these solutions is quite clear. The former (it has the same form as (37.7)) corresponds to an experiment in which a_1 and X_1 collide (an incoming wave is observed in one channel only); their collision may result in elastic scattering, described by the amplitude S_{11}, or in the reaction $a_1 + X_1 \to a_2 + X_2$, described by the amplitude S_{21} in (37.7). All the other particles with $i > 2$ may form in the interior region, but they cannot escape to infinity for lack of energy (one often says that these channels are closed). Similarly, the solution with $\alpha_1 = 0$, $\alpha_2 = 1$,

$$\Psi_2 = \psi_2^{(-)}\Phi_2 - \sum_{i=1}^{N} S_{i2}\psi_i^{(+)}\Phi_i, \tag{37.8}$$

describes physical processes which take place when the particles a_2 and X_2 collide; S_{i2} determine the interaction between particles in the entire space, including the interior region.

We thus come to the conclusion that for $Q_2 < E < Q_3$, where two channels are open (i.e., where the energy is sufficient for the existence of two pairs of particles, $a_1 + X_1$ and $a_2 + X_2$), our system has two independent wave functions satisfying the appropriate boundary conditions. Clearly, there are two and only two independent solutions, since if there were more, we could add them to Ψ_1 and Ψ_2 and thus find several different solutions with the same amplitudes α_i of the wave functions $\psi_i^{(-)}$. In this case the process would not be determined by the amplitudes of the incoming waves, i.e., in other words, the theory would not provide a single-valued description of particle collisions and thus would not be a complete theory. In any physical theory the number of independent solutions satisfying the boundary conditions is precisely equal to the number of open channels.

Now proceeding by analogy we can easily guess that further increase of energy will increase the number of independent solutions: for $Q_3 < E < Q_4$

we should have three independent wave functions, say Ψ_1, Ψ_2, and a new function

$$\Psi_3 = \psi_3^{(-)}\Phi_3 - \sum_{i=1}^{N} S_{i3}\psi_i^{(+)}\Phi_i. \tag{37.9}$$

For $Q_4 < E < Q_5$ we should have four independent solutions, etc. In general, for $Q_m < E < Q_{m+1}$, there are m independent wave functions, which can be taken in the form

$$\Psi_j = \psi_j^{(-)}\Phi_j - \sum_{i=1}^{m} S_{ij}\psi_i^{(+)}\Phi_i - \sum_{k=m+1}^{N} S_{kj}\psi_k^{(+)}\Phi_k \ (j \leqslant m). \tag{37.10}$$

The first term describes the incident wave of the particles $a_j + X_j$, the second term describes the outgoing waves of the particles $a_i + X_i$ $(i \leqslant m)$, whose creation is not forbidden by energy considerations. Finally, the third term describes the exponentially decaying "tails" of the particles $a_k + X_k$ $(k > m)$, which are formed virtually in the interior region but cannot escape to infinity for lack of energy.

The coefficients S_{ij} — the amplitudes of the function $\psi_i^{(+)}$ — are determined by the particle interaction. The most significant amplitudes are the S_{ij} of the open channels, since in terms of these amplitudes we can express the scattering and the reaction cross sections (this will be shown in what follows). These coefficients constitute the so-called scattering matrix S_{ij} S_{ij} $(i, j \leqslant m)$ (or S-matrix). It has m rows and m columns, and its order is thus precisely equal to the number of open channels. As a new channel is opened, the order of the S-matrix increases by one. The most general wave function has the form (we write out only the part corresponding to open channels)

$$\Psi = \sum_{j=1}^{m} \alpha_j \Psi_j = \sum_{j=1}^{m} \left\{ \alpha_j \psi_j^{(-)}\Phi_j - \alpha_j \sum_{i=1}^{m} S_{ij}\psi_i^{(+)}\Phi_i \right\} =$$
$$= \sum_{j=1}^{m} \Phi_j \left\{ \alpha_j \psi_j^{(-)} - \psi_j^{(+)} \sum_{i=1}^{m} \alpha_i S_{ji} \right\}. \tag{37.11}$$

Instead of writing the wave functions Φ_i of the channels, we will agree to write Ψ in the form of a column of m numbers:

$$\hat{\Psi} = \begin{pmatrix} \alpha_1\psi_1^{(-)} - \sum_i S_{1i}\alpha_i\psi_1^{(+)} \\ \alpha_2\psi_2^{(-)} - \sum_i S_{2i}\alpha_i\psi_2^{(+)} \\ \vdots \\ \alpha_m\psi_m^{(-)} - \sum_i S_{mi}\alpha_i\psi_m^{(+)} \end{pmatrix} \equiv \begin{pmatrix} \alpha_1\psi_1^{(-)} - \beta_1\psi_1^{(+)} \\ \alpha_1\psi_2^{(-)} - \beta_2\psi_2^{(+)} \\ \vdots \\ \alpha_m\psi_m^{(-)} - \beta_m\psi_m^{(+)} \end{pmatrix}, \tag{37.12}$$

where the first row is the wave function of the particles of the first channel, the second row describes the motion of particles in the second channel, etc. Introducing square $m \times m$ matrices

$$\hat{\psi}^{(\pm)} = \begin{pmatrix} \psi_1^{(\pm)} & 0 & \cdots & 0 \\ 0 & \psi_2^{(\pm)} & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & \cdots & & \psi_m^{(\pm)} \end{pmatrix}; \ \hat{S} = \begin{pmatrix} S_{11} & S_{12} & \cdots & S_{1m} \\ S_{21} & S_{22} & \cdots & S_{2m} \\ \vdots & \vdots & & \vdots \\ S_{m1} & S_{m2} & \cdots & S_{mm} \end{pmatrix} \tag{37.13}$$

and columns of coefficients before outgoing and incoming waves

$$\hat{\alpha} = \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_m \end{pmatrix}; \quad \hat{\beta} = \begin{pmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_m \end{pmatrix}, \tag{37.14}$$

we may write the matrix (37.12) in the form

$$\Psi = (\hat{\psi}^{(-)}\hat{\alpha} - \hat{\psi}^{(+)}\hat{\beta}); \; \hat{\beta} = \hat{S}\hat{\alpha}. \tag{37.15}$$

The relation between the matrices $\hat{\alpha}$ and $\hat{\beta}$, describing the amplitudes of incoming and outgoing waves, is entirely determined by the S-matrix, which thus contains all the information on the interaction properties of our system. In more precise terms, the situation is as follows. In case of potential scattering, the S-matrix degenerates to a set of numbers $S_l = e^{2i\delta_l(k)}$. In this case it has been proved /115/ that the values of all the scattering phases $\delta_l(k)$ in the entire energy range $0 < k < \infty$ completely describe the potential, i.e., the coefficients $S_l(k)$ actually contain all the information on system properties.

In multichannel systems, however, the analogous theorem has never been proved, although it seems to be self-evident. We should moreover stress that actual recovery of the system Hamiltonian from scattering data involves very substantial difficulties, partly of pure mathematical nature and partly due to the fact that we must know all the S-matrix elements at all energies. Extraction of this information from experimental data —the so-called phase analysis —requires extremely delicate experiments.

Also note another point. The general expression (37.2) shows that for $r > R$ there is a total of $2N$ independent solutions corresponding to the $2N$ constants α_l and β_l. Each of these $2N$ independent solutions can be continued into the interior region. Consider the energy interval $Q_1 < E < Q_2$. Here, as we know, there is only one physically acceptable solution. The conditions at infinity impose $(N - 1)$ constraints (37.5). One constant α_1 can be arbitrarily chosen, since it corresponds to the normalization of the wave function. There thus remain N constraints. These are the constraints imposed on the wave function in the interior region. Thus, the number of boundary conditions in the interior region is equal to the total number of channels: if there is but one channel, this condition requires that the wave function be bounded at $r = 0$. In case of N channels, the wave functions of all the channels should be regular, and this provides the N conditions in the interior region.

§ 38. CROSS SECTIONS. THE UNITARITY OF THE S-MATRIX

The S-matrix formalism is treated in considerable detail in /192/. We will therefore discuss here only the simplest case of spinless particles.

Let the energy be between $Q_m < E < Q_{m+1}$. We consider the processes taking place when the two particles a_j and X_j collide. The term corresponding to the particle pair $a_j + X_j$ in the wave function of this process is

$$\psi_j^{(-)} - S_{jj}\psi_j^{(+)} \equiv (\psi_j^{(-)} - \psi_j^{(+)}) - (S_{jj} - 1)\psi_j^{(+)} \tag{38.1}$$

(in matrix notation, this is the term occupying the j-th row). Here, as in Chapter 2, the free motion function is enclosed in the first pair of parentheses. The amplitude of the scattered wave is $S_{jj} - 1$, and the scattering cross section is

$$\sigma_{jj} = \frac{\pi}{k_j^2}(2l+1)|S_{jj} - 1|^2, \tag{38.2}$$

where the factor $\frac{\pi}{k_j^2}(2l+1)$ is associated with the fact that the plane wave

$$\frac{1}{\sqrt{v_j}} e^{(k_j r_j}$$

normalized to a current of 1 particle/sec·cm^2 contains an incoming component $\psi_j^{(-)} Y_{lm}(\theta, \varphi)$ with amplitude

$$\frac{(-1)}{k_j} i^{l-1}\sqrt{\pi(2l+1)}, \tag{38.3}$$

and the outgoing current is thus

$$\sigma_{jj} = \left|\frac{(-1)}{k_j} i^{l-1}\sqrt{\pi(2l+1)}(S_{jj} - 1)\right|^2 = \frac{\pi}{k_j^2}(2l+1)|S_{jj} - 1|^2.$$

The above expression for the scattering cross section has the same form as for potential scattering. The only difference is that for multichannel systems the matrix elements $|S_{jj}| \leqslant 1$ so that the scattering phases are complex.

Let us now compute the cross section σ_{jl} of the reaction $X_j(a_j, a_l)X_l (l \neq j)$. For unit current (1 particle/sec·cm^2) of colliding particles, the outgoing current of the pairs $a_l + X_l$ through a sphere of large radius is equal by definition to the creation cross section of these particles,

$$\sigma_{jl} = \left|\frac{1}{k_j} i^{l-1}\sqrt{\pi(2l+1)}\, S_{jl}\right|^2 = \frac{\pi}{k_j^2}(2l+1)|S_{jl}|^2. \tag{38.4}$$

Expressions (38.2) and (38.4) can be combined, writing the cross section of the reaction $X_j(a_j, a_l)X_l$ in the form

$$\sigma_{jl} = \frac{\pi}{k_j^2}(2l+1)|S_{jl} - \delta_{jl}|^2, \tag{38.5}$$

where δ_{jl} is the Kronecker delta.

The above expressions show that the cross sections of all the processes are described in terms of the S-matrix elements. A study of the general properties of the S-matrix is therefore of fundamental importance.

We will first show that the elements of the S-matrix are not independent: they satisfy certain constraints. It is clear from physical considerations

that in any physical process the total number of particles should be conserved. In other words, whatever the actual superposition of the wave functions

$$\Psi = \Sigma a_j \Psi_j, \tag{38.6}$$

the sum of the particle currents converging at the origin should be equal to the sum of the outgoing currents.

The total incoming current according to (37.11) and (37.12) is

$$I^{(-)} = \sum_{j=1}^{m} |a_j|^2,$$

and the total outgoing current (see (37.11)) is

$$I^{(+)} = \sum_{i=1}^{m} \left| \sum_{j}^{m} S_{ij} a_j \right|^2 = \sum_{jk} S_{ij} a_j S_{ik}^* a_k^*.$$

These currents should be equal for any values of the constants a_i. Equating the expressions in $I^{(-)}$ and $I^{(+)}$ for the same products $a_i a_j^*$, we obtain the constraints imposed on the S-matrix:

$$\sum_{i=1}^{m} S_{ij} S_{ik}^* = \delta_{jk}. \tag{38.7}$$

A matrix whose elements S_{ij} satisfy (38.7) is called a unitary matrix.

Thus, the law of particle number conservation leads to the unitarity of the S-matrix. In matrix form, this condition is written as

$$\hat{S}^+ \hat{S} = 1, \text{ i.e., } \hat{S}^+ = \hat{S}^{-1}, \tag{38.8}$$

where $\hat{S}^+$ is the Hermitian conjugate, i.e., a matrix obtained from $\hat{S}$ by taking the complex conjugate of the transpose. In the simplest case of a one-channel system, (38.8) reduces to the well-known condition

$$S^* S = 1.$$

§ 39. TIME REVERSAL. THE SYMMETRY OF THE S-MATRIX

The laws of classical mechanics allow time reversal. This statement should be interpreted in the following way. Consider a system of N particles whose motion is described by the coordinates and the velocities

$$x_i(t); \quad v_i(t). \tag{39.1}$$

At some time $t = T$ we arrest the motion of all the particles and make them move in the opposite direction with the velocities

$$-v_i(T).$$

If this is done, the system will go through a reverse sequence of all the stages of its previous evolution, i.e., the coordinates and the velocities for $t > T$ will be given by

$$x_i'(T+\tau) = x_i(T-\tau); \quad v_i'(T+\tau) = -v_i(T-\tau). \tag{39.2}$$

To prove this proposition, it suffices to consider the equations of motion. They have the form

$$m_i \frac{dv_i}{dt} = \sum_{j=1}^{N} F(x_i - x_j), \tag{39.3}$$

where F are the interparticle forces. Here we consider the simplest case of forces which only depend on the relative position of the particles. If (39.1) is a solution of these equations, direct substitution shows that the functions

$$v_i'(t) \equiv -v_i(-t); \quad x_i'(t) = x_i(-t) \tag{39.4}$$

are also solutions of the equations of motion (39.3). This proves the reversibility of time in classical mechanics.

In quantum mechanics the problem of time reversal is formulated as follows /193/. A wave function $\psi(x, t)$ of an evolving process should be found from the equation

$$i\hbar \frac{\partial \psi(x,t)}{\partial t} = \hat{H}\psi(x,t), \tag{39.5}$$

where x is the set of all the coordinates describing the system. At a time t the probability density and the mean momentum are

$$\left.\begin{aligned} w(x, t) &= |\psi(x, t)|^2, \\ p(t) &= \int \psi^*(x, t)\, \hat{p}\psi(x, t)\, dx. \end{aligned}\right\} \tag{39.6}$$

The principle of time reversibility states that, in parallel with any process described by the function $\psi(x, t)$, there must exist a reverse process with the wave function $\psi_{rev}(x, t)$ such that

$$w_{rev}(x, t) = w(x, -t), \; p_{rev}(t) = -p(-t). \tag{39.7}$$

Let us find the form of ψ_{rev}. Substituting $-t$ for t in (39.5) we form the complex conjugate of the resulting equation. Equation (39.5) thus takes the form

$$i\hbar \frac{\partial \psi^*(x, -t)}{\partial t} = H^* \psi^*(x, -t), \tag{39.8}$$

so that if $H^* = H$,

$$\psi_{rev}(x, t) = \psi^*(x, -t) \tag{39.9}$$

is a solution of the starting Sch. Eq. (39.5). This new solution describes the reverse process. Indeed

$$\left.\begin{aligned} w_{rev}(x,t) &= |\psi^*(x, -t)|^2 = w(x, -t), \\ p_{rev}(t) &= \int \psi(x, -t)\, \hat{p}\psi^*(x, -t)\, dx = -\left[\int \psi^*(x, -t)\, \hat{p}\psi(x, -t)\, dx\right]^* = -p(-t). \end{aligned}\right\} \tag{39.10}$$

Here we made use of the fact that by definition $\hat{p} = -i\hbar \frac{\partial}{\partial x}$, so that $\hat{p}^* = -\hat{p}$, and the mean $\boldsymbol{p}(t)$ is real.

Thus, for every process $\psi(x, t)$ there is a corresponding reverse process with the wave function $\psi_{rev}(x, t)$. A necessary condition for the existence of reverse process is that the Hamiltonian be real:

$$\hat{H}^* = \hat{H}. \tag{39.11}$$

For a system of N spinless particles with the usual potential interaction forces between them this condition is always satisfied, since the total Hamiltonian

$$\hat{H} = -\sum_{i=1}^{N} \frac{\hbar^2}{2m_i} \nabla_i^2 + \sum_{i<k} V_{ik}(r_i - r_k)$$

is real.

Some complications develop in the case of charged particles in a magnetic field. The kinetic energy operator in this case is

$$\hat{T} = \frac{1}{2m}\left(\hat{p} - \frac{e}{c} A\right)^2,$$

where A is the vector potential of the field satisfying the usual condition div $A = 0$. For $\hat{T}$ we thus have

$$\hat{T} = \frac{\hat{p}^2}{2m} + i\frac{e\hbar}{mc}(A\nabla) + \frac{1}{2m}\frac{e^2}{c^2}A^2.$$

Clearly, in distinction from the case of an electric field, the reversal of the direction of particle motion must be accompanied by a reversal of the sign of the magnetic field or, equivalently, a reversal of the sign of the vector potential. The time reversal operation should therefore contain complex conjugation and sign reversal of A (or H). We see from the expression for $\hat{T}$ that the Hamiltonian is invariant under this operation:

$$\hat{H}(A) = \hat{H}^*(-A). \tag{39.11'}$$

For a wave function $\psi_{rev}(t)$ which describes a time-inverted process we obtain as before

$$\psi_{rev}(t) = \psi^*(-t).$$

Further complications arise when dealing with particles which have spin. Consider a particle with spin of $1/2$. Its wave function is described by a column matrix

$$\psi(x, t) = \begin{pmatrix} \psi_1(x, t) \\ \psi_2(x, t) \end{pmatrix},$$

where the upper and the lower component correspond to the states with $s_z = 1/2$ and $s_z = -1/2$, respectively. The mean spin components at point x

at time t are

$$s_x = \psi^+ \hat{s}_x \psi = \frac{1}{2} (\psi_1^* \psi_2^*) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \frac{1}{2} (\psi_1 \psi_2^* + \psi_1^* \psi_2),$$
$$s_y = \psi^+ \hat{s}_y \psi = \frac{i}{2} (\psi_1 \psi_2^* - \psi_1^* \psi_2),$$
$$s_z = \psi^+ \hat{s}_z \psi = \frac{1}{2} (|\psi_1|^2 - |\psi_2|^2).$$

Hence we conclude that by passing to a complex conjugate function

$$\psi(x, t) \to \psi^*(x, t)$$

we end up with a different spin state:

$$s_x \to s_x, \quad s_y \to -s_y, \quad s_z \to s_z.$$

On the other hand, when the direction of particle motion is reversed, the angular momentum should change its sign. This is a general property of any angular momentum vector, the spin vector included. This condition is met by the function

$$\psi_{\text{rev}}(x, t) = \hat{\sigma}_y \psi^*(x, -t) = i \begin{pmatrix} -\psi_2^*(x, -t) \\ \psi_1^*(x, -t) \end{pmatrix}.$$

For the mean values of the various spin projections in this state we obtain

$$s_x'(t) = -s_x(-t); \; s_y'(t) = -s_y(-t); \; s_z'(t) = -s_z(-t).$$

The function ψ also satisfies the other reversibility conditions:
the probability density at a point x

$$w_{\text{rev}}(x, t) = (\psi_{\text{rev}}(x, t)^+ \psi_{\text{rev}}(x, t) = (|\psi_1|^2 + |\psi_2|^2) \equiv w(x, -t);$$

the mean momentum

$$p_{\text{rev}}(t) = \int dx \, \psi_{\text{rev}}^+(x, t) \hat{p} \psi_{\text{rev}}(x, t) =$$
$$= \int dx \, [\psi_2(x, -t) \hat{p} \psi_2^*(x, -t) + \psi_1(x, -t) \hat{p} \psi_1^*(x, -t)] \equiv -p(-t).$$

The function

$$\psi_{\text{rev}}(x, t) = \hat{\sigma}_y \psi^*(x, -t)$$

thus has all the properties required of the wave function describing a time-reversed process. From the equation for $\psi(x, t)$,

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = \hat{H} \psi(x, t),$$

we obtain an equation for ψ_{rev}:

$$i\hbar \frac{\partial \psi_{\text{rev}}(x, t)}{\partial t} = \hat{\sigma}_y \hat{H}^* \hat{\sigma}_y \psi_{\text{rev}}(x, t).$$

Therefore, in order for ψ_{rev} to be a solution of the Sch. Eq., or in other words for the reverse process to exist, we must have

$$\hat{H}(A) = \hat{\sigma}_y \hat{H}^*(-A)\,\hat{\sigma}_y \tag{39.11''}$$

(if there is an external magnetic field, the field sign should be reversed when the complex conjugate of the Hamiltonian is taken).

If $\hat{H}$ does not include the particle spin operator, $\hat{\sigma}_y$ and $\hat{H}$ commute: in this case the conditions of time reversibility reduce again to (39.11) and (39.11'). If $\hat{H}$ is dependent on spin, it requires special treatment. It is readily seen that an interaction of the form σH and σl, where H is the magnetic field and l is the orbital momentum operator, satisfies condition (39.11'').

This condition is not met by terms of the form σE, where E is an electric field.* The presence of these terms in the Hamiltonian indicates that the particle has an electric dipole moment $d \sim s$. Thus, as Landau first pointed out /194/, an immediate consequence of time reversibility is that a stable particle cannot have an electric dipole moment. This was the state of things up to 1964, when we had no experimental indications (or theoretical pointers) even of a remote possibility of nonreversibility of time. Thus, the discovery in 1964 of a weak breakdown of time reversibility in kaon decay experiments /94/ came as a complete surprise to the scientific world. Since there is no exact invariance under time reversal, a stable particle with spin (e.g., a proton or an electron) in general should have a small electric dipole moment.

After this brief digression, we proceed to consider the constraints imposed on the S-matrix by time reversal. The ordinary Sch. Eq. can be written in the form

$$H\psi(x) = E\psi(x). \tag{39.12}$$

Since the Hamiltonian is real, taking the complex conjugate we find that, in case of real energy, $\psi^*(x)$ is also a solution of equation (39.12). (We are dealing with spinless uncharged particles.) This consequence of the time reversal principle reveals some important properties of the S-matrix.

The asymptotic expression for the most general wave function of a multichannel system in matrix notation can be written in the form (see (37.15))

$$\hat{\Psi} \sim [\hat{\psi}^{(-)} - \hat{\psi}^{(+)}\hat{S}]. \tag{39.13}$$

On account of time reversibility, the complex conjugate function

$$\hat{\Psi}^* \sim [\hat{\psi}^{(+)} - \hat{\psi}^{(-)}\hat{S}^*] \tag{39.14}$$

is also a wave function of our system, i.e., apart from a constant factor, it should coincide with $\hat{\Psi}$. In other words, the relation between the amplitudes of the incoming and outgoing waves should be the same for both $\hat{\Psi}^*$ and $\hat{\Psi}$. Right-multiplying by $(-S^{-1})^*$ the expression in brackets in (39.14), we obtain

$$\hat{\Psi}^* \sim [\hat{\psi}^{(-)} - \hat{\psi}^{(+)}(\hat{S}^{-1})^*]. \tag{39.13'}$$

* These terms may arise only in a theory where parity is not conserved, since E is a polar and σ an axial vector, so that σE changes sign on inversion.

The relation between the amplitudes will be the same as in (39.13) if $(\hat{S}^{-1})^* = \hat{S}$. On the other hand, we know from (38.8) that $\hat{S}^{-1}=\hat{S}^+$. Therefore, recalling the definition of the matrix $\hat{S}^+$, we finally obtain

$$(\hat{S}^{-1})^* = (\hat{S}^+)^* = \hat{S}_{tr} = \hat{S}, \tag{39.15}$$

where $\hat{S}_{tr}$ is the transpose of $\hat{S}(S_{ij} \to S_{ji})$. Since by (39.15) the $\hat{S}$-matrix is not affected by transposition, it is a symmetric matrix (with $S_{ij} = S_{ji}$), so that

$$\hat{S}^+ = \hat{S}^* = \hat{S}^{-1}. \tag{39.16}$$

Time reversibility thus leads to a symmetrical scattering matrix.

In some problems, the asymptotic expression of the wave function is conveniently represented not as a superposition of incoming and outgoing waves $\psi_i^{(\pm)}$ but in the form of standing waves

$$\left.\begin{aligned} \varphi_i^{(1)} &= \frac{1}{2}(\psi_i^{(+)} + \psi_i^{(-)}) \sim \frac{1}{\sqrt{v_i}} \cos\left(k_i r - \frac{l\pi}{2}\right), \\ \varphi_i^{(2)} &= \frac{1}{2i}(\psi_i^{(+)} - \psi_i^{(-)}) \sim \frac{1}{\sqrt{v_i}} \sin\left(k_i r - \frac{l\pi}{2}\right). \end{aligned}\right\} \tag{39.17}$$

To change over from a system of wave functions (37.13) to a system of standing-wave functions, we introduce the diagonal matrices

$$\hat{\varphi}^{(1)} = \frac{1}{2}(\hat{\psi}^{(+)} + \hat{\psi}^{(-)}) \quad \text{and} \quad \hat{\varphi}^{(2)} = \frac{1}{2i}(\hat{\psi}^{(+)} - \hat{\psi}^{(-)}). \tag{39.17'}$$

We can now express $\hat{\psi}^{(\pm)}$ in terms of $\hat{\varphi}^{(1)}$ and $\hat{\varphi}^{(2)}$ and insert the resulting expression in the general wave function (39.13). We find

$$\hat{\Psi} = [\hat{\varphi}^{(1)}(1 - \hat{S}) - \hat{\varphi}^{(2)} i(1 + \hat{S})]\,\hat{\alpha} = [\hat{\varphi}^{(1)} - \hat{\varphi}^{(2)}\hat{K}]\,\hat{\gamma}. \tag{39.18}$$

where

$$\hat{K} = i(1 + \hat{S})(1 - \hat{S})^{-1}, \tag{39.19}$$

and $\hat{\gamma}$ is a new matrix of arbitrary coefficients related to the amplitude matrix $\hat{\alpha}$ of the incoming waves by the equality

$$\hat{\gamma} = (1 - \hat{S})\,\hat{\alpha}. \tag{39.20}$$

$\hat{K}$ is generally called the K-matrix and in our standing-wave representation it replaces the $\hat{S}$-matrix derived in the representation of incoming and outgoing waves. The K-matrix has a number of important properties which follow from the unitarity and symmetry of the S-matrix. To derive these properties, we right-multiply (39.19) by $(1 - \hat{S})$ and take the Hermitian conjugates of the two sides. This gives

$$(1 - \hat{S}^+)\hat{K}^+ = (1 + \hat{S}^+)(-i). \tag{39.21}$$

Further seeing that $\hat{S}^+ = \hat{S}^{-1}$, we left-multiply this equality by $\hat{S}$ and find

$$(-1 + \hat{S})\hat{K}^+ = (1 + \hat{S})(-i), \qquad (39.22)$$
$$\text{i.e., } \hat{K}^+ = i(1 + \hat{S})(1 - \hat{S})^{-1} = \hat{K}.$$

$\hat{K}$ is thus a Hermitian matrix.

As the S-matrix is symmetric, we have

$$\hat{S}^+ = \hat{S}^*. \qquad (39.23)$$

Taking the complex conjugate of (39.21) and using (39.22), (39.23), we obtain

$$(1 - \hat{S})\hat{K}^{+*} = i(1 + \hat{S}),$$

i.e.,

$$\hat{K}^* = \hat{K}^+ = \hat{K}. \qquad (39.24)$$

In other words, the K-matrix is a real and symmetric matrix. It is this simple form of the particle number conservation and the time reversibility conditions that makes the standing-wave representation particularly attractive.

Any real symmetric $m \times m$ matrix has $\frac{m(m+1)}{2}$ independent real matrix elements. The K-matrix is determined by the interaction between the particles. We may therefore say that the form of the wave function outside the interaction range depends on the particular interaction only through $\frac{m(m+1)}{2}$ real parameters. These parameters are naturally functions of energy.

If we use the standing-wave representation, these parameters are the $\frac{m(m+1)}{2}$ independent matrix elements of the K-matrix. On passing to the representation of incoming and outgoing waves, the number of independent parameters remains $\frac{m(m+1)}{2}$ as before, since the S-matrix is uniquely expressible in terms of the K-matrix. Indeed, from (39.19) we have

$$\hat{S} = (i\hat{K} + 1)(i\hat{K} - 1)^{-1}. \qquad (39.25)$$

Finally note that there are certain restrictions on the energy dependence of the S-matrix elements /191/. We will not give here the corresponding expressions, since they do not have any use.

§ 40. SOME ANALYTICAL PROPERTIES OF THE S-MATRIX

Consider a multichannel system $a_i + X_i (i = 1, 2, \ldots, N)$. Let k_1 be the wave vector of the light pair $a_1 + X_1$, x_i|the values of k_1 for which the i-th channel is open:

$$\frac{\hbar^2 x_i^2}{2m_1} = Q_i.$$

In the complex k_1 plane, the points $x_2, x_3, \ldots, x_n$ correspond to branching points of the S-matrix elements. Indeed, the elements S_{ij} of the scattering matrix depend on the wave vectors k_i of the particles in all the channels, and not only on k_1:

$$k_i = \sqrt{\frac{2m_i}{\hbar^2}(E - Q_i)}, \quad E = \frac{\hbar^2 k_1^2}{2m_1}.$$

This is most apparent from the fact that the elements S_{ij} are found by matching the "interior" with the exterior functions, whereas the latter $(\psi_i^{(\pm)})$ contain k_i and not the total energy.

Thus, in order to make S_{ij} a single-valued function of the complex variable k_1, we have to introduce cuts in the k_1 plane; these cuts will be drawn as shown in Figure 34. In the interval (Ox_2), as we know (see § 37), there is only one solution which is regular in the entire space, in the interval (x_2, x_3) there are two regular solutions, in (x_3, x_4) there are three regular solutions, etc.

Take one of the various physically meaningful solutions over the interval (x_i, x_{i+1}) (let $j \leqslant i$):

$$\Psi_j = \Phi_j \psi_j^{(-)} - \sum_{n=1}^{N} S_{jn}(k_1)\, \psi_n^{(+)} \Phi_n \sim$$
$$\sim \Phi_j \frac{1}{\sqrt{v_j}} e^{-ik_j r_j} - \sum_{n=1}^{N} S_{jn}(k_1) \frac{1}{\sqrt{v_n}} e^{ik_n r_n} \Phi_n \qquad (40.1)$$

and continue it analytically into the upper halfplane. Since the cuts have been made, this continuation is single-valued. The function $\psi_n^{(+)} \sim \frac{1}{\sqrt{v_n}} e^{ik_n r_n}$ in the upper k_1 halfplane falls off exponentially for $r \to \infty$. Hence we conclude that none of the S-matrix elements may have poles in the upper k_1 halfplane (except the poles on the imaginary axis). Indeed, let S_{ln} have a pole at a point k_r. Then divide (40.1) by S_{ln}. The resulting function is clearly regular everywhere. In the limit as $k_1 \to k_r$, this function will reduce to $\sum_{n=1}^{N} \frac{S_{jn}}{S_{ln}} \psi_n^{(+)} \Phi_n$ which by assumption is regular for all r. Thus, $\frac{\hbar^2 k_r}{2m_1}$ is an energy eigenvalue in this case. This is, however, impossible for k_r which do not lie on the imaginary axis, since otherwise the energy eigenvalue would be a complex number, at variance with the Hermitian property of the Hamiltonian. As we see from this argument, the above theorem can be extended to all the elements of the S-matrix without exception.

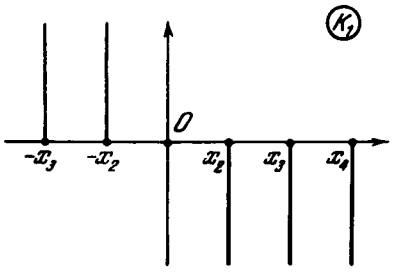

FIGURE 34.

Now suppose that there is a bound state with energy $E_0 = -\frac{\hbar^2 k_0^2}{2m_1}$ in our system. It is readily seen /195/ that at the point $k_1 = ik_0$ all the elements S_{ij} have a pole, i.e., for $k \to ik_0$ they all behave as

$$S_{ij} = \frac{C_{ij}}{k_1 - ik_0}; \quad C_{ij} = \text{const}. \qquad (40.2)$$

Indeed, $\psi_j^{(-)}$ in the upper k_1 halfplane diverges exponentially for large r. Hence, this term should drop out for $k_1 = ik_0$ when the function (40.1) is analytically continued to the imaginary axis k_1. This is possible, however, only if at least one of the elements S_{jn} goes to infinity at this point, since then the entire function ψ_j can be divided by this singular element S_{jn} and the term $\frac{1}{S_{jn}}\psi_j^{(-)}$ will vanish for $k_1 = ik_0$. On the other hand, it is clear that if at least one of the elements of the S-matrix goes to infinity, all the other elements of the S-matrix go to infinity in the same way. Indeed, the wave function of a bound state Ψ_0 should have the asymptotic form

$$\Psi_0 \sim \sum_{n=1}^{N} A_n e^{-|k_{n0}|r_n}\Phi_n, \quad |k_{n0}| = \sqrt{\frac{2m_n}{\hbar^2}(Q_n + E_0)}, \tag{40.3}$$

where the sum is taken over all the channels. Since particles from different channels may in principle transform to particles of all other channels, none of the A_n may be zero. Therefore only the term $\psi_j^{(-)}$ should drop out from the expression for the wave function when (40.1) with any j is analytically continued to the point ik_0 and in this case $\Psi_j \to \Psi_0 \cdot$ const. This is possible only if all the elements S_{jn} have the form (40.2) near the point ik_0. It is furthermore clear that for all j and n we should have

$$C_{jn} = b_j A_n \sqrt{v_n}. \tag{40.4}$$

Otherwise, using different functions ψ_j we would obtain different expressions for the wave function Ψ_0 of the bound state.

From (40.2) and (40.4) it immediately follows that the determinant assembled from the residues of the S-matrix elements and all its minors vanish at the point corresponding to a bound state.

As regards the poles of S_{jj} in the lower k_1 halfplane, they correspond to quasistationary states of the system, as in the case of the ordinary Sch. Eq.

Various analytical properties of the S-matrix are treated in /196/.

§ 41. CONSTRAINTS ON THE RESIDUES OF THE S-MATRIX ELEMENTS

In previous chapters we analyzed the properties of $S = e^{2i\delta}$ and set an upper bound for the residue of S at a point corresponding to a bound state. Similar theorems can be derived for multichannel systems.

First note that the law of particle number conservation for multichannel systems is a natural generalization of the single-channel formula:

$$\frac{\partial}{\partial t}\int_V dr\left(\sum_{j=1}^{N}|\psi_j|^2\right) = \oint_S dS\left(\sum_{j=1}^{N}\frac{i\hbar}{2m_j}(\psi_j^*\nabla\psi_j - \psi_j\nabla\psi_j^*)\right), \tag{41.1}$$

where S is the outer surface of the volume V, ψ_j is the wave function of particles in the j-th channel, m_j is the reduced mass of the particles in the j-th channel.

In matrix notation, the total wave function of the system is written as

$$\hat{\Psi} = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_N \end{pmatrix} \quad \text{and} \quad \hat{\Psi}^+ = (\psi_1^*, \psi_2^*, \ldots, \psi_N^*),$$

and expression (41.1) takes the form

$$\frac{\partial}{\partial t}\int dr \hat{\Psi}^+\hat{\Psi} = \oint_S dS \frac{i\hbar}{2}(\hat{\Psi}^+\hat{M}^{-1}\nabla\hat{\Psi} - (\nabla\hat{\Psi}^+)\hat{M}^{-1}\hat{\Psi}),$$

where

$$\hat{M}^{-1} = \begin{pmatrix} m_1^{-1} & & 0 \\ & m_2^{-1} & \\ & & \ddots \\ 0 & & m_N^{-1} \end{pmatrix}.$$

If the particles in all the channels are spinless, momentum conservation considerations indicate that transitions between channels

$$a_i + X_i \rightleftarrows a_j + X_j$$

are allowed only if the particles in the left- and the right-hand sides are in states with the same l. For simplicity, we will consider this case only.

Suppose that for a given l our multichannel system has a bound state with energy

$$E_0 = \frac{\hbar^2 k_{10}^2}{2m_1}; \quad k_{10} = ik_0$$

and normalized wave function

$$\Psi_0 = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_N \end{pmatrix} \sim e^{-\frac{iE_0 t}{\hbar}} \begin{pmatrix} A_1 e^{-|k_{10}|r} \\ A_2 e^{-|k_{20}|r} \\ \vdots \\ A_N e^{-|k_{N0}|r} \end{pmatrix}, \tag{41.2}$$

where $|k_{i0}|$ are the absolute values of the wave vectors of the particles in the i-th channel, corresponding to energy E_0.

If the k are real, the wave functions have the form

$$\Psi_j = \left(\Phi_j\psi_j^{(-)} - \sum_{i=1}^{N} S_{jl}\psi_l^{(+)}\Phi_l\right) Y_{lm}. \tag{41.3}$$

Using (41.1) —(41.3), we derive in the same way as in Chapter 3 the expression

$$S_{jj}(k_1) \xrightarrow[k_1 \to ik_0]{} \frac{(-1)^{l+1} i\,|A_j|^2}{k_j - ik_{j0}} = \frac{m_1 k_{j0}}{m_j k_{10}} \frac{(-1)^{l+1} i\,|A_j|^2}{k_1 - ik_0}, \tag{41.4}$$

which relates the residue of a diagonal element of the S-matrix to the normalization constant A_j of the bound-state wave function. Recalling

expression (40.4) of the previous section, we find

$$b_j = (-1)^{l+1} i A_j^* \frac{\sqrt{v_{j0}}}{v_{10}}, \tag{41.5}$$

where v_{j0} is the velocity corresponding to wave vector k_{j0}.

We thus arrive at a general formula

$$S_{j1}(k_1) \underset{k_1 \to ik_0}{\sim} \frac{C_{j1}}{k_1 - ik_0}, \tag{41.6}$$

where the residue C_{j1} is given by

$$C_{j1} = i(-1)^{l+1} \sqrt{\frac{v_{10} v_{j0}}{v_{10}^2}} A_1 A_j^*. \tag{41.7}$$

This is a generalization of the corresponding relation for a single-channel system (§ 15) and it sets an upper bound for the residues C_{j1}.

For simplicity, let us consider the case $l = 0$.

If the interaction range R is zero, i.e., a point interaction, expression (41.2) for the wave function of the bound state is applicable everywhere except at the point $r = 0$. The normalization condition is

$$\sum_{i=1}^{N} |A_i|^2 \frac{1}{2|k_{i0}|} = 1. \tag{41.8}$$

If all $A_i \neq 0$, we clearly have

$$|A_i|^2 < 2|k_{i0}| \tag{41.9}$$

and

$$|C_{j1}| < 2 \left| \frac{v_{10} v_{j0}}{v_{10}} \right| \frac{\sqrt{m_1 m_j}}{\hbar}. \tag{41.10}$$

Note that in distinction from a single-channel system, where for $R = 0$ we have the equality

$$|C| = 2|k_0|,$$

(41.9) is a strict inequality. The reason for this is the following: in a single-channel system the wave function comprises terms which correspond only to one pair of particles. In a multichannel system, on the other hand, Ψ_0 incorporates the particles of all the channels, so that each channel accounts for a relatively small fraction of the total wave function, a fact appropriately reflected in (41.9).

Note that scattering and reaction data, which in principle should give all the S_{j1}, can be used to find the residues C_{j1} from (41.6), (41.7) by analytical continuation of S_{j1} in the complex plane. Once the residues have been found, we can determine the normalization constants A_i. Thus, complete information on the continuum enables us to reconstruct the structure of the bound state.

If the interaction range R is finite, expression (41.2) is applicable only for $r > R$. From the normalization condition we obtain, along the same lines as in § 15, that

$$\sum_{i=1}^{N} |A_i|^2 \frac{1}{2|k_{i0}|} e^{-2|k_{i0}|R} < 1, \tag{41.11}$$

and inequalities (41.9), (41.10) are weakened:

$$|A_i|^2 < 2|k_{i0}| e^{2|k_{i0}|R}, \tag{41.12}$$

$$|C_{ij}| < 2 \left| \frac{v_{i0} v_{j0}}{v_{10}} \right| \frac{\sqrt{m_i m_j}}{\hbar} e^{(|k_{i0}|+|k_{j0}|)R}. \tag{41.13}$$

The principal consequence of this is that comparison of the experimental values of C_{ji} with inequalities (41.10), (41.13) will in principle give an estimate of the interaction range.

§ 42. EXPRESSION FOR THE S-MATRIX AND ITS RELATION TO THE R-MATRIX

In the general case of an N-channel system, the S-matrix depends on $\frac{1}{2}N(N+1)$ parameters. As a rule, we know absolutely nothing about these parameters, since particle interactions have been very little studied. We know, however, that these interactions are generally strong and of very short range. A reaction is therefore generally considered as developing in three distinct stages: 1) the particles are on collision courses, but as long as the distance between them is less than the reaction radius R, they do not interact (Coulomb forces are ignored at this conjunction); 2) for $r \leqslant R$ the interaction is turned on instantaneously and a so-called intermediate system is formed; 3) finally the intermediate system disintegrates and as soon as the distance between the product particles becomes greater than R, the interaction is instantaneously turned off.

Using this schematic picture, we can obtain fairly powerful theorems on the behavior of scattering and reaction cross sections. To this end, however, we should express the S-matrix elements in terms of the wave functions and their derivatives in the interior region $r < R$. This problem was first solved by Kapur and Peierls in 1938 /182/ and by an alternative technique by Wigner and Eisenbud in 1947 /197/. Recently Lane and Thomas /192/ published a very detailed review on this subject.

The underlying idea is the following. Consider a system with N open channels $a_i + X_i$. Outside the reaction radius, i.e., for $r > R$, transitions between channels $X_i + a_i \to X_j + a_j$ are forbidden from the very definition of reaction radius.

The most general wave function for $r > R$ is written in matrix form as

$$(\hat{\psi}^{(-)} - \hat{\psi}^{(+)}\hat{S})\,\hat{\nu} \equiv \left\{ \begin{pmatrix} \psi_1^{(-)} & & 0 \\ & \psi_2^{(-)} & \\ & \ddots & \\ 0 & & \psi_N^{(-)} \end{pmatrix} - \right. \tag{42.1}$$

$$-\begin{pmatrix} \psi_1^{(+)} & & 0 \\ & \psi_2^{(+)} & \\ & & \ddots \\ 0 & & \psi_N^{(+)} \end{pmatrix} \begin{pmatrix} S_{11}\, S_{12} \ldots \\ S_{21}\, S_{22} \ldots \\ \qquad\qquad \ddots \\ \qquad\qquad S_{NN} \end{pmatrix} \Bigg\} \begin{pmatrix} \nu_1 \\ \nu_2 \\ \vdots \\ \nu_N \end{pmatrix}, \tag{42.1}$$

where the column matrix $\hat{\nu}$ comprises arbitrary numbers ν_i, and $\psi_i^{(-)}$, $\psi_i^{(+)}$ are the wave functions describing the incoming and outgoing particles in the i-th channel.

Inside the reaction range $r < R$, there are also N regular solutions. Let their values and the values of their derivatives for $r = R$ be

$$\Psi_i = \begin{pmatrix} \alpha_{i1} \\ \alpha_{i2} \\ \vdots \\ \alpha_{iN} \end{pmatrix}, \quad \Psi_i' = \begin{pmatrix} \alpha_{i1}' \\ \alpha_{i2}' \\ \vdots \\ \alpha_{iN}' \end{pmatrix} (i = 1, 2, \ldots, N). \tag{42.2}$$

The most general solution for $r < R$ can be written as

$$\hat{\Psi}\hat{a} = \sum_{i=1}^{N} a_i \Psi_i; \quad \hat{\Psi} = \begin{pmatrix} \alpha_{11}\ \alpha_{21} \ldots \alpha_{N1} \\ \alpha_{12}\ \alpha_{22} \ldots \alpha_{N2} \\ \cdots\cdots\cdots \\ \alpha_{1N}\ \alpha_{2N} \ldots \alpha_{NN} \end{pmatrix}; \quad \hat{a} = \begin{pmatrix} a_1 \\ a_2 \\ \ldots \\ a_N \end{pmatrix}. \tag{42.3}$$

The matrix $\hat{a}$ is again quite arbitrary. We write an analogous expression for the derivative in the form

$$\hat{\Psi}'\hat{a} \equiv \sum_{i=1}^{N} a_i \Psi_i'. \tag{42.4}$$

Matching the wave functions and their derivatives at the boundary, we obtain two matrix equations

$$\left.\begin{aligned} \hat{\Psi}\hat{a} &= (\hat{\psi}^{(-)} - \hat{\psi}^{(+)}\hat{S})\,\hat{\nu}, \\ \hat{\Psi}'\hat{a} &= (\hat{\psi}^{(-)'} - \hat{\psi}^{(+)'}\hat{S})\,\hat{\nu}. \end{aligned}\right\} \tag{42.5}$$

Elementary solution gives

$$\hat{S} = (R_1\hat{\psi}^{(+)} - \hat{\psi}^{(+)'})^{-1}(\hat{R}_1\hat{\psi}^{(-)} - \hat{\psi}^{(-)'}), \tag{42.6}$$

where $\hat{R}_1$ is a square matrix,

$$\hat{R}_1 = \hat{\Psi}'\hat{\Psi}^{-1}. \tag{42.7}$$

The first part of the problem is thus completed: we have established a relation among the S-matrix and the wave function in the interior region. It now remains to find the properties of the matrix $\hat{R}_1$.

We know that the S-matrix is unitary and symmetric,

$$\hat{S}^{-1} = \hat{S}^{+}; \quad \hat{S}^{+} = \hat{S}^{*}.$$

Using these relations, we can now establish the properties of the new matrix $\hat{R}_1$. Elementary calculations show that the unitarity of the S-matrix leads to the relation

$$\hat{R}_1\hat{M} = \hat{M}\hat{R}_1^+, \tag{42.8}$$

where $\hat{M}$ is a diagonal square mass matrix

$$\hat{M} = \begin{pmatrix} m_1 & & 0 \\ & m_2 & \\ & \ddots & \\ 0 & & m_N \end{pmatrix},$$

and m_i is the reduced mass of the particles in the i-th channel. The second property of the S-matrix — its symmetry — indicates that $\hat{R}_1$ is a real matrix:

$$\hat{R}_1 = \hat{R}_1^*. \tag{42.8'}$$

At this stage we can conveniently introduce a new matrix $\hat{R}$:

$$\hat{R} = \hat{R}_1\hat{M}.$$

From the properties of $\hat{R}_1$ we see that the new matrix $\hat{R}$ is real and Hermitian. In other words, its elements are real and symmetric under index transposition:

$$R_{ik} = R_{ik}^* = R_{ki}. \tag{42.9}$$

This means that the $\hat{R}$-matrix is entirely determined by $\frac{N(N+1)}{2}$ real parameters.

In a two-channel system, say, we have three independent parameters:

$$\hat{R} = \begin{pmatrix} R_{11} & R_{12} \\ R_{12} & R_{22} \end{pmatrix}.$$

The S-matrix is thus also expressed in terms of three parameters only, but surely we know this already.

As an example, consider a two-channel system. Expression (42.6) in this case gives the following expressions for the S-matrix elements:

$$\begin{aligned}
S_{11} &= \frac{1}{Dm_1m_2}\{(R_{11}\psi_1^{(-)} - m_1\,\psi_1^{(-)\prime})\,(R_{22}\psi_2^{(+)} - m_2\,\psi_2^{(+)\prime}) - R_{12}^2\psi_1^{(-)}\psi_2^{(+)}\},\\
S_{12} &= S_{21} = -\frac{2i}{\hbar}\frac{R_{12}}{D},\\
S_{22} &= \frac{1}{Dm_1m_2}\{(R_{11}\psi_1^{(+)} - m_1\psi_1^{(+)\prime})\,(R_{22}\psi_2^{(-)} - m_2\psi_2^{(-)\prime}) - R_{12}^2\psi_1^{(+)}\psi_2^{(-)}\},\\
D &= \frac{1}{m_1m_2}\{(R_{11}\psi_1^{(+)} - m_1\psi_1^{(+)\prime})\,(R_{22}\psi_2^{(+)} - m_2\psi_2^{(+)\prime}) - R_{12}^2\psi_1^{(+)}\psi_2^{(+)}\}.
\end{aligned} \tag{42.10}$$

For a system with more than two channels, the expressions for the elements of the S-matrix are more cumbersome, but the fundamental structure is the same. They are in the form of a fraction where both

the numerator and the denominator are polynomials of N-th degree (N being the number of channels) of the exterior wave functions $\psi_i^{(\pm)}$ and their derivatives at $r = R$.

§ 43. MEAN LIFETIME OF CONTINUUM STATES

In § 35 we found the mean lifetime of a scattered particle inside a sphere of radius a where the entire potential is concentrated. We will now solve the corresponding problem for a multichannel system /200/.

Consider a system with N channels $a_i + X_i$ ($i = 1, \ldots, N$), some of which may be closed at the given energy E. Further consider one of the energetically allowed processes

$$a_i + X_i \to a_j + X_j. \tag{43.1}$$

We will now find the mean lifetime T_{ij} for this process during which the particles of the system remain inside a sphere of radius $r = a$. The radius R of the region where interchannel transitions (43.1) take place is assumed to be less than a.

We use the same timing technique as in § 35 for measuring T_{ij}: outside the spere $r = a$ there is a weak homogeneous magnetic field H directed along the z axis, and all the particles a_i ($i = 1, \ldots, N$) have a magnetic moment $\mu = \mu s$ (which is equal for all i). The colliding particles are assumed to be polarized in the direction of the x axis. Inside the interaction range the colliding particles $a_i + X_i$ may change to any other pair $a_k + X_k$, which in its turn may transform to the next pair $a_l + X_l$, etc. These transitions, however, do not affect our "clock" (i.e., the precession of the magnetic moment around the vector H), since by assumption all a_i have the same magnetic moment μ. The lifetime T_{ij} can therefore be found as

$$T = \frac{\theta}{\omega},$$

where θ is the angle between the vector μ and the x axis, which specifies the direction of the outgoing particle, and $\omega = \frac{2\mu H}{\hbar}$ is the spin precession frequency in a magnetic field.

To calculate θ, note the following. The S-matrix of the process (43.1) contains two kinds of quantities (see (42.6)): (a) the elements of the R-matrix, which depend only on particle interactions inside the reaction radius, and (b) functions $\psi_i^{(\pm)}$ and $\psi_i^{(\pm)'}$ which depend only on the behavior of particles in the various channels outside the reaction radius (note that $\psi_i^{(\pm)}$ are normalized by their asymptotic behavior

$$\psi_i^{(\pm)} \sim \frac{1}{\sqrt{v_i}} e^{\pm i\left(k_i r - \frac{l\pi}{2}\right)}.$$

In what follows we assume that the sphere of radius $r = a$ with the magnetic field inside it is the boundary separating between the interior and the exterior region.

Let the S-matrix without the magnetic field be known:*

$$\hat{S} = (\hat{\psi}^{(+)} - \hat{R}\hat{\psi}^{(+)\prime})^{-1}(\hat{\psi}^{(-)} - \hat{R}\hat{\psi}^{(-)\prime}). \tag{43.2}$$

Turning on a magnetic field inside the sphere $r = a$ is equivalent to changing the energy of the particles inside that sphere. For particles with spins aligned along $\boldsymbol{H}$ ($s_z = 1/2$) the energy E is incremented to $E + \mu H$, and for particles with spins directed against the field ($s_z = -1/2$) the energy is $(E - \mu H)$. The $\hat{R}$-matrix elements change accordingly:

$$R_{ik} \to R_{ik} \pm \mu H \frac{dR_{ik}}{dE} \quad \text{for} \quad s_z = \pm\frac{1}{2}.$$

At the same time the "exterior" functions $\psi^{(\pm)}$ are not affected by the introduction of a magnetic field at $r < a$. The S-matrix of the states with $s_z = \pm 1/2$ thus takes the form

$$\hat{S} \pm \mu H \frac{\delta\hat{S}}{\delta E} \equiv \left[\hat{\psi}^{(+)} - \left(\hat{R} \pm \mu H \frac{d\hat{R}}{dE}\right)\hat{\psi}^{(+)\prime}\right]^{-1} \times \left[\hat{\psi}^{(-)} - \left(\hat{R} \pm \mu H \frac{d\hat{R}}{dE}\right)\hat{\psi}^{(-)\prime}\right], \tag{43.3}$$

where $\frac{d}{dE}$ is the ordinary derivative with respect to energy, and $\frac{\delta}{\delta E}$ indicates that the differentiation is done assuming all the "interior" quantities to be constant.

Since the $\hat{R}$-matrix can be expressed in terms of $\hat{S}$, $\hat{\psi}^{(\pm)}$, and $\hat{\psi}^{(\pm)\prime}$ using (43.2), $\frac{\delta\hat{S}}{\delta E}$ is also expressible in terms of these quantities. Simple calculations give

$$\frac{\delta\hat{S}}{\delta E} = \frac{d\hat{S}}{dE} + \frac{d\hat{\psi}^{(+)}}{dE}(\hat{\psi}^{(+)})^{-1}\hat{S} - \hat{S}(\psi^{(-)})^{-1}\frac{d\hat{\psi}^{(-)}}{dE} - \\ - \frac{1}{2}(\hat{S} - \hat{\psi}^{(-)}(\hat{\psi}^{(+)})^{-1})\frac{d\hat{k}}{dE}\hat{k}^{-1}\hat{\psi}^{(+)}(\hat{\psi}^{(-)})^{-1}(\hat{S} + \hat{\psi}^{(-)}(\psi^{(+)})^{-1}), \tag{43.4}$$

where $\hat{k}$ is a diagonal matrix of wave vectors, and $\psi^{(\pm)}$, $\psi^{(\pm)\prime}$ should be calculated on the sphere $r = a$.

The wave function of the colliding particles $a_i + X_i$ (with μ directed along the x axis) is

$$\psi_i^{(-)}\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}.$$

The wave function of the product particles $a_l + X_l$ is clearly

$$\psi_j^{(+)}\frac{1}{\sqrt{2}}\begin{pmatrix}S_{il} + \mu H\frac{\delta S_{il}}{\delta E}\\ S_{il} - \mu H\frac{\delta S_{il}}{\delta E}\end{pmatrix} = S_{il}\psi_l^{(+)}\frac{1}{\sqrt{2}}\begin{pmatrix}1 + \mu H\frac{1}{S_{il}}\frac{\delta S_{il}}{\delta E}\\ 1 - \mu H\frac{1}{S_{il}}\frac{\delta S_{il}}{\delta E}\end{pmatrix}. \tag{43.5}$$

The angle between μ and the x axis to which this spin function corresponds is

$$\theta = 2\mu H \operatorname{Im}\left(\frac{1}{S_{il}}\frac{\delta S_{il}}{\delta E}\right).$$

* The definition of the R-matrix used here is somewhat different from that introduced in §42 /192/.

The mean lifetime T_{ll} is therefore /186/*

$$T_{ll} = \hbar \operatorname{Im}\left(\frac{1}{S_{ll}}\frac{\delta S_{ll}}{\delta E}\right). \tag{43.6}$$

In the following we will require an explicit expression for the T_{ll} of a two-channel system ($l = 0$). The S-matrix can always be written in the form

$$\hat{S} = \begin{pmatrix} \alpha e^{2i\delta_1} & i\beta e^{i(\delta_1+\delta_2)} \\ i\beta e^{i(\delta_1+\delta_2)} & \alpha e^{2i\delta_2} \end{pmatrix} \tag{43.7}$$

(this matrix is symmetric and unitary if α and β are real and $\alpha^2 + \beta^2 = 1$). Using (43.4) and (43.6), we find

$$\begin{aligned} T_{11} &= \frac{2}{v_1}\operatorname{Im}\left\{i\left(\frac{d\delta_1}{dk_1} + a\right) - \frac{1}{4k}\left(\alpha e^{2i(k_1 a+\delta_1)} - \frac{1}{\alpha}e^{-2i(k_1 a+\delta_1)}\right) + \frac{\beta^2 v_1}{4\alpha v_2 k_1}e^{2i(k_2 a+\delta_2)}\right\}, \\ T_{12} &= \hbar\left\{\frac{d}{dE}(\delta_1+\delta_2) + \alpha\left(\frac{1}{\hbar v_1} - \frac{1}{\hbar v_2}\right) - \right. \\ &\qquad \left. - \frac{\alpha}{2\hbar v_2 k_1}\sin 2(k_1 a + \delta_1) - \frac{\alpha}{2\hbar v_2 k_2}\sin 2(k_2 a + \delta_2)\right\}. \end{aligned} \tag{43.8}$$

Here k_1, v_1 and k_2, v_2 are the wave vectors and the velocities of particles in the first and the second channel, respectively. The above expression for T_{11} is applicable even in the energy range when the second channel is closed.

* A different result $T_{ll} = \hbar \operatorname{Im}\left(\frac{1}{S_{ll}}\frac{dS_{ll}}{dE}\right)$ where $\frac{d}{dE}$ is the total derivative, was obtained in some sources, e. g., /242/. In general this result is incorrect /198/, as it only corresponds to the quasiclassical approximation (but even not always so).

Chapter 7

THRESHOLD EFFECTS

Experiments show that all interactions between particles (except the Coulomb interaction) are strong but relatively short-range. This property leads to a number of important predictions concerning the cross sections of various processes. This problem was studied in the greatest detail by Wigner in 1947 /198/. He started with a multichannel system

$$a_i + X_i \to a_j + X_j$$

and showed that from the one assumption of short-range character of the nuclear forces we can compute

(a) the energy dependence of the cross sections for elastic scattering $X_i(a_i, a_i)X_i$ at low energies of incident particles;

(b) the cross sections of the reactions $X_i(a_i, a_j)X_j$ at low energies of incoming and outgoing particles.

These results were considerably extended in recent years, when the general solution was obtained for the energy dependence of the cross section of a process $X_i(a_i, a_j)X_j$ near the threshold of any other process $X_i(a_i, a_k)X_k$.

§ 44. ENERGY DEPENDENCE OF THE ELASTIC SCATTERING CROSS SECTION AT LOW ENERGIES

Let the interaction V between the particles a and X have a finite range R.

Consider a state in which a and X have a definite orbital momentum l; further let $r > R$. The Sch. Eq. for the radial part of the wave function multiplied by r, $\chi_l(r) \equiv rR_l(r)$, for $r > R$ has the form (we are dealing with neutral particles at this stage)

$$\chi''_{kl} + \left(k^2 - \frac{l(l+1)}{r^2}\right)\chi_{kl} = 0, \tag{44.1}$$

where $k = \sqrt{\frac{2mE}{\hbar^2}}$ is the wave vector of the relative motion of particles a and X, E is their energy in the center-of-mass system, and m is the reduced mass. The most general expression for χ_{kl} in this region can be written in the form

$$\chi_{kl}(r) = A_l(k)\,[\psi_l^{(-)}(kr) - S_l(k)\,\psi_l^{(+)}(kr)], \tag{44.2}$$

where A and S are certain constants dependent on k (or E) and $\psi_l^{(\pm)}$ are two solutions which at infinity have the asymptotic form of incoming and outgoing waves:

$$\psi_l^{(\pm)}(kr) = \left(\frac{\pi kr}{2}\right)^{1/2}\left[(-1)^l J_{-(l+1/2)}(kr) \pm i J_{l+1/2}(kr)\right],$$
$$\psi_l^{(\pm)}(kr) \sim \frac{1}{\sqrt{v}} e^{\pm i\left(kr - \frac{\pi l}{2}\right)}. \tag{44.3}$$

Here $J_{\pm(l+1/2)}$ are the ordinary Bessel functions. Functions normalized in this way describe the incident (−) and the outgoing (+) wave corresponding to unit current through any large sphere.

For $r = R$ the solution (44.2) should be matched continuously with the regular solution for $r < R$. In the interior region the particle energy E enters the equation of motion only as a sum $(E+V)$ with the strong (large in magnitude) nuclear interaction. The interior wave function $\chi^{(0)}$ will therefore hardly change with energy (which is small compared to V).

To first approximation we may thus take that

$$\left.\frac{\chi^{(0)\prime}}{\chi^{(0)}}\right|_{r=R} = z$$

is independent of E.

The matching condition takes the form

$$\left.\frac{\psi_l^{(-)\prime} - S\psi_l^{(+)\prime}}{\psi_l^{(-)} - S\psi_l^{(+)}}\right|_{r=R} = z \xrightarrow[k\to 0]{} \text{const.} \tag{44.4}$$

Seeing that for $k \to 0$

$$\psi_l^{(\pm)}(kr) \sim \left(\frac{\pi m}{\hbar} r\right)^{1/2}\left[\frac{(2l-1)!!}{(kr)^{l+1/2}} \pm i\frac{(kr)^{l+1/2}}{(2l+1)!!}\right], \tag{44.5}$$

we find

$$S_l - 1 = \left.\frac{\psi_l^{(-)\prime} - z\psi_l^{(-)}}{\psi_l^{(+)\prime} - z\psi_l^{(+)}}\right|_{r=R} - 1 \sim (kR)^{2l+1},$$

whence for the elastic scattering cross section as a function of energy we obtain

$$\sigma_l = (2l+1)\frac{\pi}{k^2}|S_l - 1|^2 \underset{k\to 0}{\sim} k^{4l} \sim E^{2l}, \tag{44.6}$$

i.e., for small E the neutral particles are mainly scattered in the state with zero orbital momentum. The particle cross sections with $l \neq 0$ vanish for $k \to 0$. Physically this result is quite obvious; it describes the repulsive action of the centrifugal barrier.

If a and X are electrically charged particles with charges e_1 and e_2, respectively, equation (44.1) acquires a Coulomb term

$$\chi_{kl}'' + \left[k^2 - \frac{l(l+1)}{r^2} - \frac{2m}{\hbar^2}\frac{e_1 e_2}{r}\right]\chi_{kl} = 0. \tag{44.7}$$

The general solution of this equation for $r > R$ is again written in the form (44.2); $\psi_l^{(\pm)}$, however, is now expressible in terms of the Coulomb functions:

$$\psi_l^{(\pm)}(r) = \frac{1}{\sqrt{v}}[G_l(\eta, \rho) \pm iF_l(\eta, \rho)] \sim \frac{1}{\sqrt{v}} e^{\pm i\left(kr - \frac{\pi l}{2} - \eta \ln 2kr + \eta_l\right)}, \tag{44.8}$$

where $\eta = \frac{e_1 e_2}{\hbar v}$, $\rho = kr$, G_l and F_l are the irregular and the regular Coulomb functions, respectively, and η_l is the Coulomb phase. The general solution for $r > R$ is written as

$$\psi_l = A_l[(\psi_l^{(-)} - \psi_l^{(+)}) + (1 - S_l)\psi_l^{(+)}]. \tag{44.9}$$

If A_l is taken equal to $\frac{l}{2k}\sqrt{v}(2l+1)i^l e^{i\eta_l}$, the first term will coincide with the coefficient before $P_l(\cos\theta)$ in the exact wave function describing Coulomb scattering. We know from scattering theory in a Coulomb field (see § 10) that this function contains the scattered wave (which should be multiplied by $P_l(\cos\theta)$ in order to obtain the scattering amplitude in a state with momentum l):

$$\frac{1}{2ik} e^{i(kr - \eta \ln 2kr)}(2l+1)(e^{2i\eta_l} - 1). \tag{44.10}$$

The second term in (44.9) corresponds to the additional nuclear scattering, and it must be added to (44.10) if we are to obtain the total scattered wave. For the total scattering amplitude in a state with momentum l we thus obtain

$$f_l = \frac{2l+1}{2ik}[e^{2i\eta_l} - 1 + e^{2i\eta_l}(S_l - 1)]P_l(\cos\theta). \tag{44.11}$$

For $k \to 0$ $(k > 0)$ the Coulomb functions behave as

$$\begin{aligned} F_l &\to C_l (kr)^{l+1}, \\ G_l &\to \frac{(kr)^{-l}}{(2l+1)C_l}\left[1 + 2\eta(kr)^{2l+1}\left(\frac{C_l}{C_0}\right)^2 O_l(r)\right], \end{aligned} \tag{44.12}$$

where $O_l(r)$ is a certain smooth function of k which is independent of r and is of the order of unity; also

$$C_l = C_0 \frac{2^l}{\Gamma(2l+2)}[(1^2 + \eta^2)(2^2 + \eta^2)\ldots(l^2 + \eta^2)]^{1/2}, \qquad C_0 = \left[\frac{2\pi\eta}{e^{2\pi\eta} - 1}\right]^{1/2}. \tag{44.13}$$

The matching condition (44.4) gives

$$S_l - 1 = -2i\frac{F_l}{G_l}\frac{F_l'/F_l - z}{(G_l'/G_l) - z + \frac{i}{G_l}(F_l' - zF_l)}. \tag{44.14}$$

We see from expansions (44.12) that the dominant energy dependence is represented by the factor

$$\frac{F_l}{G_l} = C_l^2 \frac{(kr)^{2l+1}(2l+1)}{1 + 2\eta(kr)^{2l+1}\left(\frac{C_l}{C_0}\right)^2 O_l(r)}\Bigg|_{r=R}. \tag{44.14'}$$

For sufficiently small k, when $\eta^2 \gg l^2$, this formula takes a simpler form, since by (44.12) and (44.13)

$$\frac{P_l}{Q_l} \approx \frac{\text{const}}{|e^{2\pi\eta}-1|}. \tag{44.15}$$

For particles of like charge, $\eta > 0$ and

$$|S_l - 1| \approx \frac{P_l}{Q_l} \approx e^{-2\pi\eta}. \tag{44.16}$$

If the particles have charge of different signs, $\eta < 0$ and

$$|S_l - 1| \approx \text{const}. \tag{44.16'}$$

Note that the right-hand sides of (44.16) and (44.16') are independent of l for $\eta^2 \gg l^2$. The physical reason for this is that the centrifugal potential ($\sim \frac{1}{r^2}$) falls off much faster than the Coulomb potential ($\frac{1}{r}$), so that the latter is the dominant factor.

The partial scattering cross section is

$$\sigma_l = \frac{\pi}{k^2}(2l+1)|(e^{2i\eta_l}-1) + e^{2i\eta_l}(S_l-1)|^2 =$$

$$= \frac{\pi}{k^2}(2l+1)\{4\sin^2\eta_l - 2\mathrm{Re}[(S_l-1)(e^{2i\eta_l}-1)] + |S_l-1|^2\} \equiv \sigma_l^c + \sigma_l^{(1)} + \sigma_l^{(2)}. \tag{44.17}$$

The first term is the pure Coulomb scattering. The Coulomb phase for small k goes to infinity:

$$\eta_l = \frac{1}{2i}\ln\frac{\Gamma(l+1+i\eta)}{\Gamma(l+1-i\eta)} \sim -\eta + \frac{\pi}{2}\left(l+\frac{1}{2}\right)\frac{\eta}{|\eta|}.$$

Therefore σ_l^c for $k \to 0$ oscillates and goes to infinity as k^{-2} for all l.

The second term in (44.17) describes the interference between nuclear and Coulomb scattering and it is also an oscillating term. To orders of magnitude,

$$\sigma_l^{(1)} \sim \begin{cases} \frac{1}{k^2}e^{-2\pi\eta} & \text{for repulsion,} \\ \frac{1}{k^2} & \text{for attraction;} \end{cases} \tag{44.18}$$

$\sigma_l^{(2)}$ — the pure nuclear part of the cross section — is a monotonic function of energy:

$$\sigma_l^{(2)} \sim \begin{cases} \frac{1}{k^2}e^{-4\pi\eta} & \text{for repulsion,} \\ \frac{1}{k^2} & \text{for attraction.} \end{cases} \tag{44.19}$$

Nuclear scattering ($\sigma_l^{(1)} + \sigma_l^{(2)}$) for particles of like charges is thus exponentially small for $k \to 0$ compared to Coulomb scattering (σ_l^c) and is entirely suppressed by the latter. In case of Coulomb attraction, all the three terms in (44.19) are of the same order of magnitude.

A characteristic feature of (44.18) and (44.19) is that neither contains l. This is true for $\eta^2 \gg l^2$, which is equivalent to the condition

$$E \ll \left(\frac{e_1 e_2}{R}\right)^2 \Big/ \frac{\hbar^2 l^2}{mR^2}. \tag{44.20}$$

At higher energies, expressions (44.18) and (44.19) are inapplicable for a given l.

§ 45. ENERGY DEPENDENCE OF TWO-PARTICLE REACTION CROSS SECTIONS FOR LOW ENERGIES OF INCOMING OR OUTGOING PARTICLES

Consider the case when the collision of two particles a and X is not restricted to simple scattering; the two particles may also react,

$$a + X \to b + Y, \tag{45.1}$$

producing two new particles b and Y. As before, we will first treat the case of neutral spinless particles. Let r be the distance between a and X, r_1 the distance between b and Y. Outside the interaction range, the wave function of the system in a state with momentum l should have the form (we use the same notation as before)

$$A_l\{[\psi^{(-)}_{k,l}(r) - S_l\psi^{(+)}_{k,l}(r)]\,\Phi(a,X) - M_l\varphi^{(+)}_{k_2 l}(r_1)\,\Phi(b,Y)\}, \tag{45.2}$$

where the expression in brackets describes the incident and the scattered waves of the pair $a + X$ (see (44.2)), and the last term describes the outgoing wave attributable to the product particles $b + Y$. $\Phi(i,j)$ is formed as the product of the interior wave functions of particles i and j. Here M_l is some function of k, and $\varphi^{(+)}_{k_2 l}$ is that solution of the Sch. Eq. for the particles $b + Y$* which behaves asymptotically as

$$\varphi^{(+)}_{k_2 l}(r_1) \sim \frac{1}{\sqrt{v_2}} e^{i\left(k_2 r_1 - \frac{l\pi}{2}\right)}$$

(k_2 and v_2 are the wave vector and the velocity of the particles $b + Y$). The exact expression for $\psi^{(+)}_l$ is given by (44.3), where r_1 should be substituted for r, k_2 for k, and m_1 (the reduced mass of the pair $b + Y$) for m.

Consider the case of a reaction which absorbs energy ($Q > 0$), i.e., which may occur only if the energy of the particles $a + X$ (in the CM system) is such that $E > Q$. The energy of the product particles $b + Y$ in this case is $E - Q$, and k_2 and v_2 are given by

$$k_2 = \sqrt{\frac{2m_1(E-Q)}{\hbar^2}}; \quad v_2 = \frac{k_2\hbar}{m_1}. \tag{45.3}$$

* Note that the Sch. Eq. is applicable to these particles only if the distance between them is $r_1 > R$, i.e., the particles are free. For $r_1 < R$ the particles $b + Y$ cannot be treated separately from $a + X$, since there is a possibility of transitions $a + X \rightleftarrows b + Y$ and the system is described by a more complex equation.

The wave function (45.2) at $r_1 = R$ should match continuously the interior wave function, and the constants S_l and M_l are determined from this condition. The interior function is unknown, since we did not specify any particular interaction. We are certain, however, that this is a bounded function. In other words, at $r = R$ the product $M_l \varphi_{k_2 l}^{(+)}(R)$ is also bounded. For $k_2 \to 0$, $\varphi_l^{(+)} \sim k_2^{-(l+1/2)}$, and for the product to be bounded we should have

$$M_l(k_2) \sim \frac{1}{\varphi_{k_2 l}^{(+)}(R)} \sim k_2^{l+1/2}. \tag{45.4}$$

The reaction cross section

$$\sigma_l^{(\text{reac})} = \frac{\pi}{k_2^2}(2l+1)\,|M_l|^2 \underset{k_2 \to 0}{\sim} k_2^{2l+1}. \tag{45.5}$$

Thus, near the creation threshold, two slow neutral particles are created in a state with $l = 0$.

Let us now find the energy dependence of the reverse reaction

$$b + Y \to a + X \tag{45.6}$$

for low energies E_1 of the particles $b + Y$. The cross section of this reaction, as we know, is

$$\sigma_l^{(\text{rev})} = \frac{\pi}{k_1^2}(2l+1)\,|M_l|^2$$

and it is determined by the same scattering matrix element M_l as the direct reaction. For the energy dependence we thus obtain

$$\sigma_l^{(\text{rev})} \underset{k_2 \to 0}{\sim} k_2^{2l-1}. \tag{45.7}$$

For small k_1 the reaction mainly occurs in the state with $l = 0$ and the reaction cross section is

$$\sigma_0 \sim \frac{1}{k_2}. \tag{45.8}$$

This is the famous "$1/v$ law" which describes the energy dependence of the cross section of nuclei for the capture of slow neutrons.

Since the state with $l = 0$ is dominant, the cross sections for absorption or creation of slow particles are spherically symmetric.

The energy dependences (45.5)—(45.7) are determined entirely by the form of the wave functions $\varphi_l^{(+)}$ of the slow particles in a state with given orbital momentum and by the boundedness condition imposed on the system wave function; these expressions are independent of the properties of the fast particles. In particular, a and X may even be charged particles.

The situation entirely changes, however, if the slow particles are charged.

In this case $\varphi_l^{(+)}$ is expressible in terms of Coulomb functions:

$$\varphi_l^{(+)} = \frac{1}{\sqrt{v_2}}(G_l + iF_l)$$

and using (44.12), (44.13) we obtain:

for the reaction X (a, b) Y (production of slow charged particles)

$$\sigma_l^{(\text{reac})} = \frac{\pi}{k_1^2}(2l+1)|M_l|^2 \sim \frac{1}{k_1^2}\frac{1}{|\varphi_l^{(+)}|^2} \sim \\ \sim \begin{cases} e^{-2\pi\eta}, & \text{if } b \text{ and } Y \text{ have like charges,} \\ \text{const}, & \text{if } b \text{ and } Y \text{ have unlike charges;} \end{cases} \tag{45.9}$$

for the reaction Y (b, a) X (collision of slow charged particles)

$$\sigma_l \sim \frac{1}{k_2^2}\frac{1}{|\varphi_l^{(+)}|^2} \sim \begin{cases} \frac{1}{k_2^2}e^{-2\pi\eta}, & \text{if } b \text{ and } Y \text{ have like charges,} \\ \frac{1}{k_2^2}, & \text{if } b \text{ and } Y \text{ have unlike charges.} \end{cases} \tag{45.10}$$

The condition of applicability of these expressions is the same as for elastic scattering of charged particles ((44.20) of the previous section). A characteristic feature is that σ_l are independent of l for $\eta^2 \gg l^2$. The reason for this is the same as before: the Coulomb barrier is much "wider" than the centrifugal barrier, so that the latter is relatively insignificant for low energies. If the particles b and Y have like charges, their capture and creation cross sections are exponentially small and the fact that σ_l is independent of l is of no particular significance.

If, however, the particles have unlike charges, the position changes since the cross sections σ_l with $l \neq 0$ are by no means small and even at very low energies the reaction comprises numerous partial waves. The cross section thus retains a definite angular anisotropy up to the very lowest energies, unlike the cross sections of neutral particles.

Another remarkable feature of the production cross sections of slow particles of unlike charges is that the cross section is finite starting at the very threshold. At the threshold the cross section thus abruptly and discontinuously falls to zero. Of course, in reality there is no such jump. The point is that production of charged particles is accompanied by emission of γ quanta and introduction of this factor, as was shown by V.M. Galitskii, leads to a very steep but nevertheless smooth (and not discontinuous) drop of the cross section to zero as $k_1 \to 0$. The cross section thus very rapidly increases as we move away from the threshold, approaching a constant value.

For easy reference, we have summarized all the results of this and previous sections in Tables 1 and 2 below.

TABLE 1. Scattering of slow particles

No Coulomb interaction between a and X	a and X have like charges	a and X have unlike charges
	$\sigma_l = \sigma_l^c + \sigma_l^{(1)} + \sigma_l^{(2)}$	$\sigma_l^c = \frac{4\pi}{k^2}\sin^2\eta_l$
$\sigma_l \sim k^{4l}$	$\sigma_l^{(1)} \sim k^{-2}e^{-2\pi\eta}$ (oscillating factor) $\sigma_l^{(2)} \sim k^{-2}e^{-4\pi\eta}$	$\sigma_l^{(1)} \sim k^{-2}$ (oscillating factor) $\sigma_l^{(2)} \sim k^{-2}$

All the results of this and previous sections are applicable if the nuclear interaction V falls off sufficiently fast with distance. It can be shown that a sufficient condition is exponential decrease of the interaction

$$V \underset{r\to\infty}{\sim} e^{-\alpha r}$$

with arbitrarily small parameter α. In what follows we invariably assume that this condition is satisfied, but in most practical cases a weaker constraint will be quite adequate as well.

TABLE 2. Reactions with the participation of slow particles b Y and fast particles a X

	No Coulomb interaction between b and Y	b and Y have like charges	b and Y have unlike charges
$Y(b, a)X$	$\sigma_l \sim k_2^{2l-1}$	$\sigma_l \sim k_2^{-2} e^{-2\pi\eta}$	$\sigma_l \sim k_2^{-2}$
$X(a, b)Y$	$\sigma_l \sim k_2^{2l+1}$	$\sigma_l \sim e^{-2\pi\eta}$	$\sigma_l \sim$ const

We have so far regarded b and Y as spinless particles. The above results, however, are entirely determined by the form of the radial wave functions and are independent of the spin functions. Therefore all the threshold energy features (Tables 1 and 2) can be immediately extended to the case of particles with spin.

With regard to the applicability of these expressions, we would like to mention the following:

(a) in their derivation we assumed that the quantities (of the type of z in (44.4)) associated with the interior region ($r < R$) were independent of energy;

(b) for the exterior wave functions we used their asymptotic expressions (44.5) and (44.12).

The first of these two assumptions has a direct bearing to the particular problem being considered, and it should naturally be verified in each case.

As regards the second assumption, we can be more definite in our evaluation:

1) expansions (44.5) are applicable for $k_1 R \ll 1$, i.e., they are valid for energies

$$(\Delta E)_a \ll \frac{\hbar^2}{2mR^2}$$

near the threshold;

2) expansions (44.12) are valid for

$$(\Delta E)_b \ll \left(\frac{e_1 e_2}{R}\right)^2 \Big/ \frac{\hbar^2 l^2}{2mR^2}.$$

Sometimes, e.g., in the case of charged "strange" particles, we have

$$(\Delta E)_a \gg (\Delta E)_b.$$

This gives rise to the following remarkable situation: immediately near the threshold ($E_1 < (\Delta E)_b$) all the energy dependences are of the "Coulomb" type. However, for $(\Delta E)_b < E < (\Delta E)_a$, the Coulomb interaction is ignorable and the cross sections behave as those of neutral particles

§ 46. ENERGY DEPENDENCE OF THE $X\,(a, a)\,X$ SCATTERING CROSS SECTION NEAR THE $X\,(a, b)\,Y$ THRESHOLD, WHEN X, a, b, Y ARE SPINLESS NEUTRAL PARTICLES

We will now show that the elastic scattering cross section has a very peculiar energy dependence near the threshold of the reaction $X\,(a, b)\,Y$ /198–200/. The four possible energy curves are shown in Figure 35. Analysis of these curves yields a wealth of information on spins and parities of the particles X, a, b, Y and on their interactions.

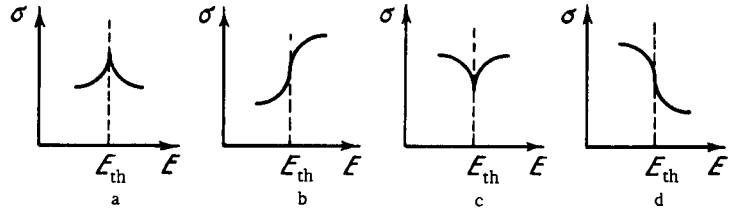

FIGURE 35.

Suppose that when the relative energy E of the particles X and a is less than E_{th}, only elastic scattering $X\,(a, a)X$ is allowed, whereas for $E > E_{th}$ the reaction $X\,(a, b)\,Y$ is also possible and the wave function thus has the asymptotic form

$$\left[e^{ik_1 r} + \frac{1}{r} e^{ik_1 r} \sum_l \frac{2l+1}{2ik_1} (S_l - 1) P_l\right] \Phi(a, X) + \\ + \frac{e^{ik_2 r_1}}{2ik_2 r_1} \sum_l (2l+1) M_l P_l \Phi(b, Y) \sqrt{\frac{v_1}{v_2}}. \qquad (46.1)$$

Here $\Phi(i, k)$ are the interior wave functions of a pair of particles i and k; k_1 and k_2 are the wave vectors of the relative motion of the pairs a, X and b, Y; v_1 and v_2 are the corresponding velocities, and P_l is the Legendre polynomial. The first term in (46.1) describes elastic scattering and the last term accounts for the reaction. The matrix elements of scattering and of the reaction S_l and M_l are related by the unitarity condition

$$|S_l|^2 + |M_l|^2 = 1, \qquad (46.2)$$

Below the threshold, the particles b, Y cannot escape to infinity for lack of energy. The last term in (46.1) in this case describes exponentially decaying "tails": k_2 is imaginary, $k_2 = i|k_2|$, and $e^{ik_2r_1} = e^{-|k_2|r_1}$. The law of particle number conservation (i.e., equality of incoming and outgoing currents) has the form

$$|S_l|^2 = 1. \tag{46.2'}$$

As we have seen in the previous section, the reaction cross section near the threshold depends on energy as

$$\sigma_l^{(\text{react})} = \frac{\pi}{k_1^2}(2l+1)|M_l|^2 \sim k_2^{2l+1},$$

so that $M_l = m_l k_2^{l+1/2}$, where m_l is a constant. Inserting this expression in (46.2), we find for $E > E_{\text{th}}$

$$|S_l| \approx 1 - \tfrac{1}{2}|m_l|^2 k_2^{2l+1}, \tag{46.3}$$

i.e.,

$$S_l = S_l^{(0)}\left(1 - \tfrac{1}{2}|m_l|^2 k_2^{2l+1}\right), \tag{46.3'}$$

where $|S_l^{(0)}| = 1$. The matrix element S_l is an analytic function of energy, and expansion (46.3') should therefore remain valid for $E < E_{\text{th}}$, where no inelastic processes occur and where $|S_l| = 1$. Since below the threshold k_2 is imaginary, then at least up to terms of the order k_2^{2l+1} we again have below the threshold $|S_l^{(0)}| = 1$. The equality $|S_l^{(0)}| = 1$ is thus applicable both above and below the threshold, so that $S_l^{(0)}$ may be written as $e^{2i\delta_l^{(0)}}$, where the phase $\delta_l^{(0)}$ is real both above and below the threshold, i.e., for both real and imaginary k_2. This means that $\delta_l^{(0)}$ contains only even powers of k_2:

$$\delta_l^{(0)}(k_2) = \delta_l^{(0)}(0) + k_2^2 a + \ldots$$

Immediately near the threshold ($k_2 R \ll 1$, where R is the reaction radius), we can drop all powers of k_2 higher than the first, so that

$$S_0(k) = e^{2i\delta_0}\left(1 - \tfrac{1}{2}|m_0|^2 k_2\right);\ S_l(k) = e^{2i\delta_l}, \tag{46.4}$$

where δ_l is the value of the phase $\delta_l^{(0)}$ at the threshold. Thus, near the threshold all S_l with $l \neq 0$ can be treated as constant, whereas S_0 is a linear function of k_2.

Given the energy dependence of S_l, we can compute the energy variation of the elastic scattering cross section near the threshold:

$$\begin{aligned}\sigma_{\text{el}}(\theta, E) = |f(\theta, E)|^2 &= \left|f(\theta, E_{\text{th}}) - \frac{1}{4ik_1}e^{2i\delta_0}|m_0|^2 k_2\right|^2 = \\ &= \sigma_{\text{el}}(\theta, E_{\text{th}}) - \frac{k_1}{2\pi}\sqrt{\sigma_{\text{el}}(\theta, E_{\text{th}})\,\sigma_{\text{i}}(|k_2|)} \times \\ &\quad \times \begin{cases}\sin(2\delta_0 - \alpha) & \text{for } E > E_{\text{th}}, \\ \cos(2\delta_0 - \alpha) & \text{for } E < E_{\text{th}}.\end{cases}\end{aligned} \tag{46.5}$$

Here $\sigma_{el}(\theta, E_{th})$ is the differential cross section for the elastic scattering $X(a, a)X$ at the threshold, $\alpha = \alpha(\theta)$ is the phase of the scattering amplitude at $E = E_{th}$:

$$f(\theta, E_{th}) = e^{i\alpha(\theta)} |f(\theta, E_{th})|,$$

and $\sigma_i(|k_2|) = \frac{\pi}{k^2}|m_0|^2 k_2$ coincides with the total reaction cross section if $E > E_{th}$

Near the threshold $\sigma_i(|k_2|)$ is proportional to $|k_2|$ and all the other terms are independent of energy. Thus near the threshold $\sigma_{el}(\theta, E)$ is a linear function of $|k_2| \sim \sqrt{|E - E_{th}|}$; the various forms of energy curves are shown in Figure 35.

Note another important point which will often recur in the following: the form of the elastic scattering cross section near threshold contains a wealth of information on the properties of our system.

Indeed, the cross section σ_{el} is a linear function of $|k_2|$ on either side of the threshold. Measuring the slope factors of the two branches and assuming the cross section $\sigma(\theta, E_{th})$ at the threshold to be known, we can use (46.5) to calculate $2\delta_0 - \alpha(\theta)$ and the reaction cross section $\sigma_i(|k_2|)$. Since, moreover, we know the value of

$$|f(\theta, E_{th})| = \sqrt{\sigma_{el}(\theta, E_{th})},$$

we can find the function

$$e^{-2i\delta_0} f(\theta, E_{th}) \equiv e^{-i(2\delta_0 - \alpha)} |f(\theta, E_{th})|,$$

whose expansion in Legendre polynomials directly gives all the scattering phases δ_l. It is readily seen that no ambiguities and uncertainties arise in this case, which generally plague the ordinary phase analysis where they are eliminated only if the scattering cross sections are known for all energies from 0 to ∞.

For the total elastic scattering cross section we have from (46.5)

$$\sigma_{el}(E) = \sigma_{el}(E_{th}) - 2\sigma_i(|k_2|) \begin{cases} \sin^2\delta_0 & \text{for } E > E_{th}, \\ \frac{1}{2}\sin 2\delta_0 & \text{for } E < E_{th}, \end{cases} \qquad (46.5')$$

i.e., only two types of energy curves are possible in this case (types a and b in Figure 35).

The range of application of (46.5) and (46.5') is determined by natural constraints which follow from our derivation: the reaction matrix element M_0 should be proportional to $k_2^{1/2}$, and its square should be small, $|M_0|^2 \ll 1$. Both these conditions are satisfied if $k_2 R \ll 1$, which in fact determines the energy range around the threshold where (46.5) and (46.5') apply:

$$k_2 \ll \frac{1}{R}, \text{ i.e., } \sqrt{|E - E_{th}|} \ll \sqrt{\frac{\hbar^2}{2mR^2}}. \qquad (46.6)$$

Another condition is that the intermediate system should have no resonances near the threshold, since otherwise the resonance phase δ_0 is a rapidly varying function of energy and the expansion analogous to (46.5) will be very complex.

§ 47. PHYSICS OF EFFECTS NEAR THE THRESHOLD OF AN INELASTIC CHANNEL

Let us consider the physics of our result. Formally, the threshold is a singular (branching) point of the equation describing the properties of our system, since for $E < E_{th}$ this equation has a unique solution corresponding to the scattering $X(a, a)X$, whereas above the threshold ($E > E_{th}$) there are two independent solutions corresponding to different conditions at infinity: 1) the particles a, X collide and 2) the particles b, Y collide. It is therefore clear that at the threshold the wave function of the system has a singularity. The physical character of this singularity can be easily elucidated by considering the asymptotic expression for the wave function (46.1). Below the threshold the particles b, Y produced in collision between a, X cannot separate for lack of energy. Outside the reaction range their probability density decreases exponentially,

$$|M_0|^2 |\varphi_{b,Y}|^2 dr \approx e^{-2|k_2|r_1} |m_0|^2 \left(\frac{m_{b,Y}}{\hbar}\right) dr_1. \qquad (47.1)$$

As we approach the threshold, $k_2 \to 0$ and the "cloud" of the particles b, Y, whose distribution in space is proportional to $e^{-2|k_2|r}$, spreads over progressively larger distances from the reaction region. In other words, the radius of the intermediate state produced by collision between a, X and the relative number of b, Y particles in this intermediate state increase indefinitely as we approach the threshold. The lifetime of the intermediate state increases correspondingly.

When we cross the threshold, the exponential tails $e^{-|k_2|r_1}$ become outgoing waves ($e^{i|k_2|r_1}$) of particles b, Y, so that free particles b, Y may exist for $E > E_{th}$.

Thus, the immediate reason for threshold anomalies is to be sought in the indefinite "swelling" of the intermediate system as we approach the threshold from below.

This qualitative conclusion can be confirmed by a direct calculation /187/ from (43.8) of the time T_{11} that the system remains in a sphere of radius $r = R_1$, where R_1 is greater than the particle interaction range.

The scattering matrix can be written as

$$\hat{S} = \begin{pmatrix} \alpha e^{2i\delta_1} & i\beta e^{i(\delta_1+\delta_2)} \\ i\beta e^{i(\delta_1+\delta_2)} & \alpha e^{2i\delta_2} \end{pmatrix}.$$

We know from the preceding analysis that
for $E > E_{th}$

$$\alpha = (1 - \gamma k_2), \quad \beta = (2\gamma k_2)^{1/2}, \quad \delta_2 = \nu k_2, \quad \delta_1 = \delta_{10},$$

for $E < E_{th}$

$$\alpha = 1, \ \delta_1 = \delta_{10} - \frac{1}{2}\gamma |k_2|, \ \delta_2 = i\nu |k_2|, \ \beta^2 = i2\gamma |k_2|,$$

where δ_{10}, $\gamma = \frac{1}{2}|m_0|^2$, and ν are constants.

Inserting in (43.8), we find that below the threshold

$$T_{11}(R_1, E) - \frac{2R_1}{v_1} = \left\{\frac{\gamma}{\hbar |v_2|}\left(1 - e^{-2|k_2|(R_1+\nu)}\right) - \frac{1}{k_1 v_1}\sin 2(k_1 R_1 + \delta_1)\right\}, \qquad (47.2)$$

and above the threshold

$$T_{11}(R_1, E) - \frac{2R_1}{v_1} = \left\{ -\frac{1}{k_1 v_1} \sin 2(k_1 R_1 + \delta_1) + \frac{\gamma}{v_2} \sin 2k_2 (R_1 + \nu) \right\}. \qquad (47.3)$$

The only rapidly varying functions of energy in these expressions are $|v_2|$ and $|k_2|$. The energy dependence $T_{11}(R_1, E)$ below the threshold is thus entirely determined by the first term in (47.2). For fixed R_1 this term monotonically increases as we approach the threshold. The qualitative trend of T_{11} as a function of energy is shown in Figure 36. T_{11} has its maximum at the threshold point.

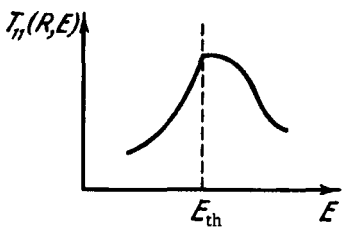

FIGURE 36.

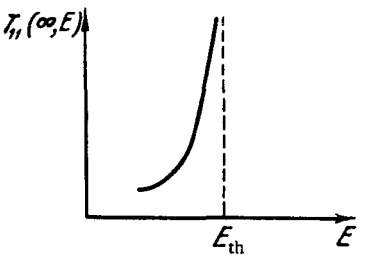

FIGURE 37.

Expressions (47.2), (47.3) give the time $T_{11}(R_1, E)$ that the system spends inside a sphere $r = R_1$. We have already seen, however, that the radius of the intermediate system increases indefinitely (as $\frac{1}{|k_2|}$) on approaching the threshold. Therefore $T_{11}(R_1, E)$ must be less than the true lifetime of the intermediate state.

To establish the energy dependence of the true lifetime, we should take $R_1 \gg \frac{1}{|k_2|}$. In this case, as the energy is incremented by ΔE, the time that the system spends inside a sphere $r = R_1$ changes by

$$(T_{11}(R_1, E + \Delta E) - T_{11}(R_1, E)) \underset{R_1 \to \infty}{\to} \gamma \left(\frac{1}{|v_2'|} - \frac{1}{|v_2|} \right), \qquad (47.4)$$

where $|v_2'|$ is the magnitude of the velocity corresponding to the energy $E + \Delta E$. Clearly, expression (47.4) gives the energy dependence of the true lifetime of the intermediate state near the threshold. We see that on approaching the threshold from below the true lifetime of the intermediate state goes to infinity as $\sim \frac{1}{\sqrt{E_{th} - E}}$ (Figure 37). This is consistent with the qualitative treatment at the beginning of this section.

§ 48. GENERALIZATION TO PARTICLES WITH SPIN

In previous sections we already observed that the study of threshold anomalies in cross sections provides a wealth of information on system properties. This is particularly clear for particles with spin.

Consider two most important cases, which will help us to elucidate all the characteristic features arising when particles with spin are involved /201/.

Let a and X be spinless particles, let Y have a spin s and let b have a spin of one half. Two cases are possible:

(a) $P(a)P(X) = P(b)P(Y)$ ($P(i)$ is the parity of the particle i). Near the threshold b and Y are created in a state with orbital momentum $l = 0$, i.e., total momentum $j = s \pm 1/2$. Since by assumption the parity of the incoming and the product particles is the same, the reaction $X(a, b)Y$ is possible only if $a+X$ have an even orbital momentum l_1 equal either to $s+1/2$ or $s-1/2$ (according as which of the two numbers is even). Correspondingly, condition (46.2) will relate M_0 to S_{l_1} and not S_0, and in place of (46.4) we obtain

$$S_{l_1} = e^{2i\delta_{l_1}}\left(1 - \frac{1}{2}|m_0|^3 k_2\right); \quad S_l = e^{2i\delta_l} \quad (l \neq l_1).$$

The scattering cross section now takes the form

$$\sigma_{el}(\theta, E) = \sigma_{el}(\theta, E_{th}) - \frac{k_1}{2\pi}\sqrt{\sigma_{el}(\theta, E_{th})}\,\sigma_t(|k_2|)(2l_1+1)\times \\ \times P_{l_1}(\cos\theta)\begin{cases}\sin(2\delta_{l_1}-\alpha) & \text{for } E > E_{th}\\ \cos(2\delta_{l_1}-\alpha) & \text{for } E < E_{th}\end{cases} \qquad (48.1)$$

and we see that the cross section anomaly described by the second term in this formula vanishes for those angles when $P_{l_1} = 0$. We can thus find the orbital momentum l_1 and hence the spin of the particle Y.

(b) The case $P(a)P(X) = -P(b)P(Y)$ differs from the previous case in that l_1 is now odd. Since $P_{2n+1}(\cos\frac{\pi}{2}) = 0$ and $P_{2n}(\cos\frac{\pi}{2}) \neq 0$, if the threshold anomaly vanishes for $\theta = \frac{\pi}{2}$ (in the CM system) we can safely say that the initial and the final particles had different parities, whereas if the threshold anomaly does not vanish at that angle, the parities were the same.

Study of threshold anomalies, as we see from (48.1), gives various other data as well:

1) the ratio of slope factors of the cross section curve before and after the threshold gives $(2\delta_{l_1} - \alpha(\theta))$;

2) the angular distribution gives the modulus of the scattering amplitude $|f(\theta, E_{th})|$;

3) the angular distribution of the anomalous term in (48.1) then gives the orbital momentum l_1 and hence all the elastic scattering phases;

4) the magnitude of the anomaly gives the total reaction cross section σ_1;

5) the parity and the angular momentum l_1 give an indication of the relative parities of the pairs a, X and b, Y and determine the spin of the particle Y. This method of parity determination is particularly promising in the physics of "strange" particles.

Thus, detailed study of the elastic cross section near the threshold greatly facilitates the very problem of phase analysis, makes it uniquely solvable, and supplies a wealth of information on the inelastic channel as well.

If the spin of particle b is some j, and not $1/2$, the only complication is that the anomalous term in (48.1) will have to be replaced by a sum of identical terms corresponding to all the values of l_1 allowed by momentum and parity conservation. This will make the analysis more tedious, but in no way affect the amount of data that can be extracted from experimental scattering findings.

Another important case is when the incident particles also have spin. Let a have spin $1/2$ and X be spinless, as before; the spins of b and Y are $1/2$ and s, as before.

The finite spin of a introduces a substantial complication in the relevant expressions, since now for the two values of the total momentum $j = s \pm 1/2$ of the product particles we have to find two orbital momenta l_1 and l_2 of the pair a, X of appropriate parity such that the corresponding total momenta $j_1 = l_1 \pm 1/2$ and $j_2 = l_2 \pm 1/2$ are equal to $s + 1/2$ and $s - 1/2$, respectively. Thus, the reaction may proceed through any of the two orbital states and it is therefore described by two matrix elements $M_{s+1/2} \equiv M'$, $M_{s-1/2} \equiv M''$. The linear dependence on k_1 near the threshold is therefore characteristic of two orbital states:

$$S_{l_1}^{s+1/2} = e^{2i\delta_{l_1}^{s+1/2}}\left(1 - \frac{k_2}{2}|m'|^2\right); \quad S_{l_2}^{s-1/2} = e^{2i\delta_{l_2}^{s-1/2}}\left(1 - \frac{k_2}{2}|m''|^2\right). \tag{48.2}$$

Now the previous formulas can be easily applied to calculate the cross section and the polarization of a, X:

$$\left.\begin{aligned} &\sigma_{el}(\theta, E) = |g(\theta, E)|^2 + |h(\theta, E)|^2, \\ &\mathcal{P}(\theta, E) = 2\,\mathrm{Im}\,[h(\theta, E)\, g^*(\theta, E)]/\sigma_{el}(\theta, E), \\ &g(\theta, E) = \frac{1}{2ik_1}\sum_l [(l+1)(S_l^{l+1/2} - 1) + l(S_l^{l-1/2} - 1)]\, P_l, \\ &h(\theta, E) = \frac{1}{2ik_1}\sum_l [S_l^{l-1/2} - S_l^{l+1/2}]\, P_l^{(1)}. \end{aligned}\right\} \tag{48.3}$$

If, say, the internal parity of the particles before and after the reaction is the same and s is odd, all the S_l^j near the threshold can be treated as constant, except

$$S_{l_1}^{l_1-1/2} = e^{2i\delta_{l_1}^{l_1-1/2}}\left(1 - \frac{k_2}{2}|m'|^2\right), \quad l_1 = s+1,$$

$$S_{l_2}^{l_2+1/2} = e^{2i\delta_{l_2}^{l_2+1/2}}\left(1 - \frac{k_2}{2}|m''|^2\right), \quad l_2 = s-1,$$

and by (48.3) we have

$$\begin{aligned} g(\theta, E) &= g(\theta, E_{th}) + \frac{ik_2}{k_1}\left[|m'|^2 l_1 e^{2i\delta_{l_1}^{l_1-1/2}} P_{l_1} + |m''|^2 (l_2+1) e^{2i\delta_{l_2}^{l_2+1/2}} P_{l_2}\right], \\ h(\theta, E) &= h(\theta, E_{th}) - \frac{ik_2}{k_1}\left[|m'|^2 e^{2i\delta_{l_1}^{l_1-1/2}} P_{l_1}^{(1)} + |m''|^2 e^{2i\delta_{l_2}^{l_2+1/2}} P_{l_2}^{(1)}\right], \end{aligned} \tag{48.4}$$

where, as before, k_1 and k_2 are the wave vectors of the relative motion of particles aX and bY, respectively, and $P_l^{(1)}$ is the associated Legendre polynomial. Inserting (48.4) in (48.3), we readily obtain the energy dependence of the cross section and the polarization. Both are found to have a singularity at the threshold, as expected. The cross section and the polarization are both linear functions of $|k_2|$ near the threshold, so that experiments at a fixed angle θ give six quantities: $\sigma_{el}(\theta, E_{th})$, $\mathcal{P}(\theta, E_{th})$, and the slope factors of σ and $\mathcal{P}$ on either side of the threshold. Analysis of the experimental data is not as simple as before, but it nevertheless gives the parity and the spin of Y, the cross sections $\sigma_l^{s\pm1/2}$, and the elastic scattering phases δ_l^j.

Threshold measurements give such a wealth of information for a fairly simple reason. Near the threshold, we actually measure three independent quantities: the relevant parameter itself (cross section, polarization, etc.) and its derivatives with respect to $|k_2|$ on either side of the threshold, which

are expressible in terms of the scattering phases at the threshold. Thus, near the threshold the experiment yields three times as much data for the determination of the unknowns as the usual experiments do.

Suppose, for example, that particle a (spin 1/2) is scattered off X (spin 0). If in the relevant energy range all the inelastic channels are closed, it is well known that phase analysis requires measurement of the cross section and the polarization of a at all angles. If, however, some inelastic channels are open, phase analysis can be made only if, besides the elastic channel, we have investigated all the open inelastic channels. Even in this case the phase analysis does not give single-valued results. The situation therefore is substantially simpler if we study the region near one of the thresholds.

Suppose that this is the first threshold, i.e., for $E < E_{th}$ only elastic scattering is possible. By measuring the cross section below and above the threshold, we obtain three equations for the scattering phases. Thus, polarization measurement is superfluous, since from the three equations provided by the measurements of σ we can find all the phases δ_l^j and hence to compute the polarization (in ordinary cases we have only two equations for phases: the measured values of σ and $\mathcal{P}$). In the more complex case when several inelastic channels are open and the scattering phases are complex numbers, cross section and polarization measurements near the threshold will enable us to determine all the phases without going into a long study of all the open channels besides the elastic channel.

Threshold regions are thus unique in the sense that relatively simple means are sufficient to disclose a wealth of information there.

§ 49. GENERALIZATION TO THE MULTICHANNEL CASE

We have so far considered only two coupled channels (a,X and b,Y). In practice, however, we are often dealing with multichannel problems. A suitable example is provided by most nuclear reactions and also by reactions between strange particles. We will therefore consider the general case of a multichannel system /201/. We start with $N+1$ pairs of particles a_i, X_i ($i = 1, 2, \ldots, N+1$), which may react according to the general scheme

$$a_i + X_i \rightleftarrows a_j + X_j.$$

Let the channels be numbered in the order of increasing threshold energies E_i (i.e., the lowest rest energy is that of the channel a_1, X_1; as the energy is increased, the channel a_2, X_2 is opened, and so on). The properties of this system are described by a $(N+1)$-row scattering matrix S_{ij} ($i, j = 1, 2, \ldots, N+1$).

Let us study the energy dependence of the scattering matrix elements near the threshold of the $(N+1)$-th channel. The cross section of the $i \to j$ process is $\sigma_{ij} = \frac{\pi}{k_i^2} |S_{ij} - \delta_{ij}|^2$, where k_i is the wave vector in the i-th channel (we assume for simplicity that all the particles are neutral and spinless and further consider only the case of zero orbital momentum. The generalization to finite spins and orbital momenta is trivial, though fairly tedious.)

Near the $(N+1)$-th channel all the $S_{i(N+1)}$ have the form $S_{i(N+1)} = m_i k^{1/2}$; $S_{N+1,\,N+1} = 1$, where m_i are constants and $k \equiv k_{N+1}$.

The law of particle number conservation leads to unitarity of the S-matrix, i.e., the matrix elements are related by

$$\sum_{k=1}^{N+1} S_{ik} S_{lk}^{*} = \delta_{il}, \tag{49.1}$$

where the dummy index goes over all the open channels. Time reversibility makes the S-matrix symmetric:

$$S_{ik} = S_{ki}. \tag{49.2}$$

Using these general properties and the known form of $S_{i(N+1)}$, we can find the energy dependence of all the matrix elements S_{ij} near the threshold of the $(N+1)$-th channel. We expand all S_{ij} with $i, j \neq N+1$ in powers of k (retaining only the first two terms):

$$S_{ij} = S_{ij}^{(0)} + a_{ij} k. \tag{49.3}$$

Since all S_{ij} are analytic functions, this expansion is valid both above and below the $(N+1)$-th threshold. Below the threshold, there are N open channels, k is imaginary ($k = i|k|$), and the unitarity condition takes the form

$$\sum_{l=1}^{N} (S_{il}^{(0)} + a_{il}\, i|k|)(S_{ml}^{(0)*} - a_{ml}^{*}\, i|k|) = \delta_{im}. \tag{49.4}$$

At the threshold ($k = 0$) it reduces to

$$\sum_{l=1}^{N} S_{il}^{(0)} S_{ml}^{(0)*} = \delta_{im}, \tag{49.5}$$

Above the threshold ($k = |k|$), a new channel has been opened and the unitarity condition is

$$\sum_{l=1}^{N} (S_{il}^{(0)} + a_{il} k)(S_{ml}^{(0)*} + a_{ml}^{*} k) + m_i m_m^{*} k = \delta_{im}. \tag{49.6}$$

From all these equalities, we obtain by elementary manipulations the following expressions for the coefficients a_{ij}:

$$a_{ij} = -\frac{1}{2} m_i m_j. \tag{49.7}$$

This is the solution of the problem formulated at the beginning of this section. Indeed, it enables us to find the energy dependence of all the cross sections σ_{ij} near the threshold of the $(N+1)$-th channel (note that to simplify the treatment we confined ourselves to the case of zero orbital momentum):

$$\sigma_{ij} = \frac{\pi}{k_i^2} |S_{ij} - \delta_{ij}|^2 = \sigma_{ij}(E_{N+1}) + \frac{\pi}{k_i^2} \operatorname{Re}[(\delta_{ij} - S_{ij}^{(0)*}) m_i m_j k] =$$

$$= \sigma_{ij}(E_{N+1}) + \frac{\pi}{k_i^2} |k| \begin{cases} \operatorname{Re}[(\delta_{ij} - S_{ij}^{(0)*}) m_i m_j] & \text{for } E > E_{N+1}, \\ -\operatorname{Im}[(\delta_{ij} - S_{ij}^{(0)*}) m_i m_j] & \text{for } E < E_{N+1}, \end{cases} \tag{49.8}$$

m_i and m_j, apart from phase factors, are proportional to the square root of $\sigma_{i(N+1)}k^{-1}$ and $\sigma_{j(N+1)}k^{-1}$, respectively.

Thus the threshold anomaly of the $i \to j$ process increases with increasing cross section or, in other words, as the coupling $i \to (N+1)$ and $j \to (N+1)$ become stronger. This opens immense vistas for the study of interactions between any pair of particles from the energy dependence of the reaction between other particles.

The fundamental conclusion can be summarized as follows. At the threshold the cross sections of all the processes $i \to j$ have singularities of the form shown in Figure 36. Study of these singularities will disclose a wealth of information.

§ 50. SINGULARITIES NEAR THE CREATION THRESHOLD OF CHARGED PARTICLES

We have seen that the magnitude of threshold singularities in the cross section of the elastic scattering $X(a, a)X$ increases with increasing cross section of the threshold process $X(a, b)Y$. For this reason, the only contribution to singularities near the creation threshold of uncharged particles comes from the b, Y creation channel in a state with $l = 0$, since for $l \neq 0$ the creation reaction is suppressed: the centrifugal barrier prevents the product particles b and Y from leaving the reaction region.

If the particles b and Y have like charges, their creation cross section near the threshold is small even in the channel with $l = 0$ on account of the Coulomb barrier. No threshold singularities will thus be observed in the elastic cross section in this case.

The position is entirely different if b and Y are particles of unlike charge, and this case deserves special attention /202/. The approach outlined in § 46 is inapplicable in this case: for neutral b and Y the threshold point $E = E_{th}$ is a simple branching point and the expansion for S obtained above the threshold remains valid below the threshold as well, which is no longer so for charged b and Y. The point E_{th} in this case is an essential singularity, since in a Coulomb field there is an infinite number of bound states with E_{th} as their condensation point. The expansions of all the physical quantities below and above the threshold are now essentially different. A more detailed analysis of the problem is therefore indicated. We will have to introduce a number of assumptions concerning the properties of our system, since the principle of particle number conservation in itself is no longer sufficient.

In what follows we assume that all the particle interactions (except the Coulomb forces) are zero outside a certain range R, which is referred to as the reaction range or radius. This assumption alone is sufficient to establish the form of threshold singularities.

We know from the general theory of reactions that outside the reaction radius the wave function of the reaction

$$a + X \begin{cases} \nearrow a + X \\ \searrow b + Y \end{cases}$$

has the form (we consider only one partial state at this stage, and therefore only the radial part is given)

$$\Psi = [\psi^{(-)} - S_{aa}\psi^{(+)}]\Phi(a, X) - S_{ab}\varphi^{(+)}\Phi(b, Y), \tag{50.1}$$

$\psi^{(\pm)}$ are the radial functions of particles $a + X$ which have the asymptotic form $\sim \frac{1}{\sqrt{v_a}} e^{\pm ikr}$, $\varphi^{(+)}$ is the radial function of particles $b + Y$,

$$\varphi^{(+)} = \frac{1}{\sqrt{v_b}}(G + iF);$$

S_{aa} and S_{ab} are the elements of the scattering matrix.

We know from the previous chapter that in two-channel systems the scattering matrix elements depend on the interaction inside the reaction range ($r < R$) only through three real parameters. In terms of these parameters, the relevant elements of the S-matrix can be written in the form (see footnote to p. 168)

$$\left.\begin{aligned} S_{aa} &= \frac{\psi^{(-)}(1 - R_{aa}\tau_a^*)(1 - R_{bb}\tau) - R_{ab}^2\tau_a^*\tau}{\psi^{(+)}(1 - R_{aa}\tau_a)(1 - R_{bb}\tau) - R_{ab}^2\tau_a\tau}, \\ S_{ab} &= \frac{2iR(k_a k)^{1/2}}{\psi^{(+)}\varphi^{(+)}} \cdot \frac{R_{ab}}{(1 - R_{aa}\tau_a)(1 - R_{bb}\tau) - R_{ab}^2\tau_a\tau} \end{aligned}\right\}. \tag{50.2}$$

Here $\tau_a = \left.\frac{\psi^{(+)'}}{\psi^{(+)}}\right|_{r=R}$; $\tau = \left.\frac{\varphi^{(+)'}}{\varphi^{(+)}}\right|_{r=R}$ are the logarithmic derivatives of the wave functions at the reaction radius, k is the wave vector of the pair $b + Y$, R_{lk} are the "interior" constants (the elements of the R-matrix) which are determined by the nature of the interaction for $r \leqslant R$; R_{lk}, $\psi^{(\pm)}$, and τ_a can be regarded as virtually constant since $\varphi^{(+)}$ and τ are extremely sensitive to energy (E_n is an ordinary regular point for R_{lk}, $\psi^{(\pm)}$, and τ_a, whereas for φ and τ this is an essential singularity). We may therefore write (50.2) in the form

$$S_{aa} = e^{2i\delta}\frac{1 - \tau/\Delta^*}{1 - \tau/\Delta}; \quad S_{ab} = \frac{k^{1/2}}{\varphi^{(+)}}\frac{C}{\Delta - \tau}, \tag{50.2'}$$

where all the slowly varying quantities are collected in the constants δ, C, and Δ, so that the dependence on the "fast" variables τ and $\varphi^{(+)}$ emerges distinctly. The matrix elements S_{ab} and S_{aa} naturally satisfy the unitarity condition which in this case is equivalent to the statement that δ is real and $\operatorname{Im}\Delta = -\left|\frac{C}{2}\right|^2$.

To find the energy dependence of the elastic cross section, we require the logarithmic derivative of τ above and below the threshold. This derivative cannot be computed using expressions (44.12) of this chapter, as they are applicable only above the threshold, when $k > 0$. We have to use the general expression for the Coulomb function, which remains valid below the threshold as well:

$$\varphi_{kl}^{(+)}(r) = \frac{1}{\sqrt{v}} e^{i\varkappa\eta - \frac{\pi\eta}{2} - i\frac{l\pi}{2}} \sqrt{\Gamma(l + 1 + i\eta)\Gamma(l + 1 - i\eta)} \times$$
$$\times \frac{1}{\Gamma(2l + 2)}\left(-\frac{\sin\pi(l + 1 + i\eta)}{\pi}\right) e^{ikr} r^{l+1} \times \tag{50.3}$$

$$\times \left\{ \ln z \sum_{s=0}^{\infty} \frac{z^s}{\Gamma(s+1)} \frac{\Gamma(q+s)\Gamma(p)}{\Gamma(q)\Gamma(p+s)} + \right.$$
$$+ \sum_{s=0}^{\infty} z^s \frac{\Gamma(p)}{\Gamma(p+s)\Gamma(s+1)} \frac{\Gamma(q+s)}{\Gamma(q)} \times [\psi(q+s) - \psi(p+s) - \psi(s+1)] +$$
$$\left. + \sum_{s=1}^{p-1} (-1)^{s+1} \frac{1}{z^s} \frac{\Gamma(s)\Gamma(q-s)\Gamma(p)}{\Gamma(q)\Gamma(p-s)} \right\}. \qquad (50.3)$$

Here $z = -2ikr$; $q = l + 1 + i\eta$; $p = 2l + 2$, Γ is the gamma function, and ψ is its logarithmic derivative. Above the threshold ($k > 0$), the function $\varphi_{kl}^{(+)}$ reduces to

$$\frac{1}{\sqrt{v}}(G_{kl} + iF_{kl}).$$

For $|k| \to 0$, $r \to 0$, we obtain from (50.3) the following approximate expression for τ:

$$\tau_{kl} \approx \frac{l+1}{r}\left\{1 - \frac{2l+1}{l+1}\frac{1}{1+\zeta l}\right\}, \qquad (50.4)$$

where ζ is an energy-independent constant,

$$\zeta = \frac{\pi(2k\eta)^{2l+1}}{(2l+1)\Gamma^2(2l+1)}, \qquad (50.4')$$

and

$$t = \frac{1}{\pi}[\ln(-2ikr) + \psi(l+1+i\eta) - \ln|2k\eta r|].$$

In case of particles of unlike charges, $\eta = \frac{e_1 e_2}{\hbar v} < 0$ above the threshold; below the threshold, where $v = i|v|$, $i\eta < 0$. Seeing that for large values of the argument the function ψ behaves as

$$\psi(w) \underset{|w|\to\infty}{\sim} \ln w$$

for nonnegative w and as

$$\psi(w) \underset{|w|\to\infty}{\sim} \ln(-w) - \pi \cot \pi w$$

for negative w, we obtain

$$t \underset{|\eta|\to\infty}{\sim} \begin{cases} l & \text{for } E > E_{\text{th}}, \\ (-1)^l \cot i\pi\eta & \text{for } E < E_{\text{th}}. \end{cases} \qquad (50.5)$$

Above the threshold t is constant, whereas below the threshold it goes to infinity an infinite number of times:

$$(-1)^l \cot i\pi\eta = (-1)^{l+1} \cot \pi \sqrt{\frac{e_1^2 e_2^2 m}{2\hbar^2 (E_{\text{th}} - E)}}.$$

The energies E_n at which the cotangent is infinite are given by

$$E_{\text{th}} - E_n = \frac{1}{n^2} \frac{e_1^2 e_2^2 m}{2\hbar}, \qquad (50.6)$$

where n is an integer. This expression coincides with the expression for the energy of the Coulomb bound states of the pair $b + Y$, which would have existed had the only forces between b and Y been Coulomb forces.

Let us now consider the behavior of the elastic cross section. The matrix element S_{aa} can be written as

$$S_{aa} = \frac{\alpha + \beta\zeta^l}{\alpha^* + \beta^*\zeta^l} = S_l,$$

where $\alpha = \alpha_1 + i\alpha_2$ and $\beta = \beta_1 + i\beta_2$ are complex constants formed in an obvious way from the constants Δ and δ in (50.2') and the constants entering expression (50.4) for τ.

Above the threshold $t = i$ and the cross section of the $X(a, a)X$ scattering is

$$\sigma_s = \frac{\pi}{k_a^2}(2l+1)|S_l - 1|^2 = \frac{\pi}{k_a^2}(2l+1)\left|\frac{\alpha + i\zeta\beta}{\alpha^* + i\zeta\beta^*} - 1\right|^2. \tag{50.7}$$

The cross section of the reaction $X(a, b)Y$ is

$$\sigma_r = \frac{\pi}{k_a^2}(2l+1)(1 - |S_l|^2) = \frac{\pi}{k_a^2}(2l+1)\left\{1 - \left|\frac{\alpha + i\zeta\beta}{\alpha^* + i\zeta\beta^*}\right|^2\right\}. \tag{50.8}$$

Both cross sections are independent of energy since k_a — the wave vector of the pair $a + X$ — can be regarded as constant near the threshold.

Below the threshold only elastic scattering is allowed. Its cross section has an infinite number of resonances which have the threshold as their condensation point:

$$\sigma_s = \frac{\pi}{k_a^2}(2l+1)|S_l - 1|^2 = \frac{2\pi}{k_a^2}(2l+1)(1 - \operatorname{Re} S_l) = \frac{4\pi}{k_a^2}(2l+1)\sin^2\delta_l,$$

$$\delta_l = \tan^{-1}\frac{\alpha_2 + \beta_2(-1)^{l+1}\zeta\cot\pi\sqrt{\frac{e_1^2e_2^2m}{2\hbar^2|E - E_{th}|}}}{\alpha_1 + \beta_1(-1)^{l+1}\zeta\cot\pi\sqrt{\frac{e_1^2e_2^2m}{2\hbar^2|E - E_{th}|}}}. \tag{50.9'}$$

The physical reason for the appearance of resonances is the following. If the particles $b + Y$ were not coupled with the $a + X$ channel and there were only Coulomb interaction forces between them, the energies (50.6) would correspond to bound states of the $b + Y$ pair. The coupling with the $a + X$ channel makes these states unstable with respect to decay into $a + X$.

The $X(a, a)X$ cross section develops resonances corresponding to these quasistationary states. The position of these resonances is determined by the condition $\delta = n\pi + \frac{\pi}{2}$, whence we obtain

$$\cot\pi\sqrt{\frac{e_1^2e_2^2m}{2\hbar^2(E_n - E_r)}} = (-1)^l\frac{1}{\zeta}\frac{\alpha_1}{\beta_1}. \tag{50.10}$$

This condition does not coincide with (50.6), i.e., the resonances are somewhat shifted relative to the position of the hydrogen-like levels (50.6). This is quite proper, since the Coulomb forces are not the only forces acting between b and Y.

The density of levels $\rho(E)$ (the number of resonances per unit energy interval) calculated from (50.10) is

$$\rho(E) = \frac{1}{2}\sqrt{\frac{e_1^2 e_2^2 m}{2\hbar^2}}\frac{1}{(E_{\text{th}} - E)^{1/4}}; \tag{50.11}$$

it increases as we come nearer the threshold. On the other hand, the cross section averaged over some interval $2\Delta E$,

$$\bar{\sigma}_s = \frac{1}{2\Delta E}\int_{E-\Delta E}^{E+\Delta E} dE\sigma_s(E) = \frac{2\pi}{k_a^2}(2l+1)\times$$

$$\times \operatorname{Re}\left\{\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{dy}{1+y^2}\left[1 - \frac{\alpha+\beta\zeta_0 y}{\alpha^*+\beta^*\zeta y}\right]\right\} = \frac{2\pi}{k_a^2}(2l+1)\left[1 - \operatorname{Re}\frac{\alpha+i\beta\zeta}{\alpha^*+i\beta^*\zeta}\right], \tag{50.12}$$

is found to be independent of energy. This indicates that the width of the levels decreases as $(E_{\text{th}} - E)^{1/4}$ as we approach the threshold. When carrying out the integration in (50.12) we should remember that for $|S_l| < 1$, $i(\alpha\beta^* - \alpha^*\beta) > 0$.

Note that the energy-averaged cross section is continuous: comparison of (50.12) with (50.7), (50.8) shows that $\bar{\sigma}_s = \sigma_t$, where $\sigma_t = \sigma_s + \sigma_r$ is the total cross section above the threshold. * The qualitative behavior of the cross sections near the threshold is shown in Figure 38.

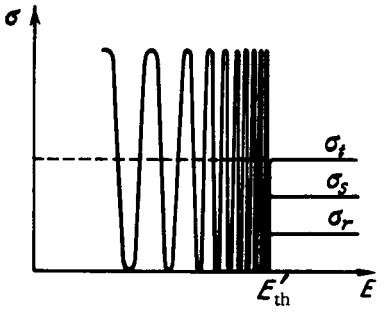

FIGURE 38.

Note that as l increases, the levels become narrower and the position of the resonances approaches the points prescribed by expression (50.6) for pure Coulomb levels. The physical reason for this is that for $l \gg 1$ the probability of finding the particles one near the other is very low, so that the transition $b + Y \to a + X$ is improbable. Thus, the lifetime of the quasistationary states increases with increasing l, and this leads to a decrease in level width. Quantitative estimates can be obtained from (50.10) noting that as l increases the constant rapidly drops to zero.

The energy interval δE where the scattering cross section has a resonance can be estimated without difficulty. It should be of the same order of magnitude as the binding energy of the first Coulomb level of $b + Y$, i.e.,

$$\delta E \approx mc^2\left(\frac{e_1 e_2}{\hbar c}\right)^2. \tag{50.13}$$

For "strange" particles $\delta E \approx 10$ MeV, so that all the specific Coulomb effects are manifested in this relatively narrow interval. At the same time the condition $kR \ll 1$ is satisfied in an interval of a few tens of MeV around the threshold. It is therefore clear that although in the immediate vicinity of the threshold the dominant effects are Coulomb effects, somewhat farther away the theory of the previous sections for neutral particles can be safely used.

* This is a natural result, since highly excited states in a Coulomb field are similar in many respects to continuum states of low positive energy. Using this analogy for averaged cross sections of processes which eventually produce highly excited atoms ($n \gg 1$), we find $\int\overline{\sigma_{nlm}}dE \sim \sigma_0 E_0/n^5$, which enables us, for example, to improve on the estimates of dielectron recombination probability derived in /243–245/.

In atomic physics the situation is reversed: the region with $kR \ll 1$ is markedly less than δE.

We have so far assumed that the system has only two open channels. The principal results can be readily generalized to the multichannel case. This can be done by replacing the expressions for the S-matrix by more general relations derived for multichannel systems. These expressions are fairly cumbersome and we do not give them here. It suffices to note that the physics remains the same: the singularities are just like in the case of a two-channel system and they are observed in the cross sections of all the processes $X_l(a_i, a_j)X_l$ which are allowed near the threshold.

Spins are also introduced without any difficulty, and add nothing new.

The theory of this section is particularly useful for the study of atomic collisions near charge exchange threshold of the form $A + B \to A^+ + B^-$ or in atomic photoeffect reactions $A + \gamma \to e^- + A^+$ near the ionization threshold. The existence of cross section resonances which have the threshold as their condensation point has been experimentally established for these cases a long time ago.

Another example is the scattering of muons by nuclei near the muon inelastic scattering threshold. Experiments with μ^- mesons may prove of particular interest, since the position and the form of the threshold resonance in the μ^- scattering cross section will enable us to gauge with considerable accuracy the deviation of the potential from the pure Coulomb potential, i.e., to measure the geometry of charge distribution in the nucleus.

Chapter 8

THE LEE MODEL

§ 51. INTRODUCTION. THE MOMENTUM REPRESENTATION

Nonrelativistic quantum mechanics (to which the scope of our book is confined) is generally concerned with the motion of particles in some given force field. Creation and transformation processes are the subject of the relativistic theory or, as it is sometimes called, the theory of quantized fields.

This "delegation of responsibility" has deep-lying roots, since when a new particle is created its energy need not be particularly close to its rest mass. In the general case particles with $E - mc^2 \sim mc^2$ are created, and these are relativistic particles.

Study of the creation of particle-antiparticle pairs draws heavily upon the relativistic form of the theory. The nonrelativistic theory of particle creation and transformation therefore cannot pretend to immediate physical applications (we are not concerned here with the many-body problem, where the concept of quasiparticles describing collective excitations is introduced). However, the nonrelativistic theory may be of certain pedagogical interest.

A student of relativistic theory has to plunge into a sea of new concepts: the definition of probability density is changed, the concept of antiparticles is introduced, Lorentz-invariance of the theory must be considered, the light cone acquires new significance, matching between theory and observations requires mass and charge renormalization, the problem of the "Moscow zero charge" is encountered.

In the nonrelativistic theory of particle creation, which is in the nature of an idealized model, on the other hand, we can calmly and quietly concentrate on the physical meaning of only some of these new and difficult concepts. Experience fully justifies this gradual approach if not for all, then at least for the majority of physicists; a notable exception was the late L. D. Landau, who was highly suspicious of all kinds of models.

A particular model of this kind was developed in some detail by Lee /203/* and it aroused considerable interest. In this chapter we consider Lee's model with some modifications. Lee started with three types of particles: two heavy particles V and N, and a light particle θ. For the

* Note that a computation technique similar to that of Lee's model had been previously used by Dirac /62/ in his analysis of resonance scattering. The modified Lee model was studied in /204, 205/. A relativistic solvable model was considered by Zachariasen /206/ and Thirring /207/.

light particle Lee uses the relativistic equation $E^2 = c^2p^2 + m^2c^4$. The antiparticle $\bar{\theta}$, however, is not considered, and this is a highly significant omission: it is particularly because of the absence of antiparticles that we may consider only few different states of N, namely either $V \rightleftarrows N + \theta$ or $\theta + V \rightleftarrows N + 2\theta$. If antiparticles are introduced, we have to consider an infinite sequence of states

$$N \rightleftarrows V + \bar{\theta} \rightleftarrows N + \theta + \bar{\theta} \rightleftarrows V + \theta + 2\bar{\theta} \rightleftarrows \ldots$$

By ignoring the antiparticle $\bar{\theta}$, the theory is confined to finite calculations.

If, however, the antiparticles $\bar{\theta}$ are ignored, the relativistic approximation for θ is superfluous and outright inconsistent.

We will therefore develop a theory in which θ is also nonrelativistic:

$$E_\theta(k) = m_\theta + \frac{k^2}{2m_\theta}. \ *$$

This theory is physically meaningful if the mass difference between N and V particles is close to the mass of θ:

$$m_V - m_N - m_\theta \ll m_\theta.$$

In this case, in addition to the usual momentum representation of the theory of fields, we can write all the results in the coordinate representations.

For the wave function of θ we can write the Sch. Eq. The creation of θ is accounted for by the inhomogeneity in the Sch. Eq., i.e., by a term not containing ψ_θ. This lends a new intuitive dimension to the theory, which is particularly helpful in connection with mass and charge renormalization.

The Lee model is also generalized to the case of N and V with spin. In this case, the theory with changing space parity leads to a relation between the spin of the unstable particle and the direction of the outgoing decay product /208/.

Apart from their educational importance, model considerations are also of heuristic value, for prediction of qualitatively new effects attributable to the interaction with electromagnetic field in theory where space parity is not conserved. This includes the dipole moment of an unstable particle /209, 210/ and the anapole moment /211, 212/ (interaction with currents) of a stable particle.

Consider a system comprising heavy particles N and V and light particles θ. The Hamiltonian of the system without interactions is the sum of the three Hamiltonians of free motion for each of the particles:

$$H_0 = \int \left[m_0 V^+(r)\, V(r) + \frac{1}{2m_0} \nabla V^+ \nabla V \right] dr + \\ + \int \left[m_N N^+(r)\, N(r) + \frac{1}{2m_N} \nabla N^+ \nabla N \right] dr + \\ + \int \left[\mu \varphi^+(r)\, \varphi(r) + \frac{1}{2\mu} \nabla \varphi^+ \nabla \varphi \right] dr. \qquad (51.1)$$

Here m_0, m_N and μ, V^+, N^+ and φ^+, V, N and φ are the rest masses and the creation and destruction operators of the particles V, N, and θ, respectively.

* Throughout this chapter we use the system of units with $\hbar = c = 1$.

Detailed discussion of the properties of these operators can be found in Landau and Lifshitz's "Quantum Mechanics" /8/.

Fourier-transforming, we change over to the momentum representation. Using the new operators, which are functions of the momentum, we write the Hamiltonian in the form

$$H_0 = \sum_k [E_V(k) V_k^+ V_k + E_N(k) N_k^+ N_k + E_\theta(k) \varphi_k^+ \varphi_k]. \tag{51.2}$$

The sum over k can be replaced in the usual way by an integral over k:

$$H_0 = \int dk\, [E_V(k) V_k^+ V_k + E_N(k) N_k^+ N_k + E_\theta(k) \varphi_k^+ \varphi_k]. \tag{51.2'}$$

Here

$$E(k) = m + \frac{k^2}{2m}. \tag{51.3}$$

Clearly, for a given momentum k, the kinetic energy of the heavy particles is ignorable compared to the kinetic energy of the light particle θ. Therefore, in what follows, we will use the Hamiltonian

$$\begin{aligned} H_0 &= \int \left[m_0 V^+(r) V(r) + m_N N^+(r) N(r) + \mu \varphi^+(r) \varphi(r) + \frac{1}{2\mu} \nabla\varphi^+ \nabla\varphi\right] dr = \\ &= \int dk \left[m_0 V_k^+ V_k + m_N N_k^+ N_k + \left(\mu + \frac{k^2}{2\mu}\right) \varphi_k^+ \varphi_k\right] \end{aligned} \tag{51.4}$$

and sometimes drop the subscript k of the operators N_k, V_k, and φ_k for simplicity. Thus, unlike Lee, we assume a nonrelativistic dependence of energy on momentum for the light particle θ, although the rest mass has been added.

The eigenvectors of H_0 can be classified according to the number of particles of each of the three different kinds. The vacuum vector $|0\rangle$ is an eigenvector of this Hamiltonian, and the corresponding energy eigenvalue is $E = 0$. Other eigenvectors are $V_k^+|0\rangle$, $N_k^+|0\rangle$, and $\varphi_k^+|0\rangle$ with the energies $E = m_0$, $E = m_N$, and $E = \mu + \frac{k^2}{2\mu}$, respectively. *

Note that all these vectors are normalized to $\delta(k - k')$:

$$\langle 0 | \varphi_{k'}, \varphi_k^+ | 0\rangle = \langle 0 | [\varphi_{k'}, \varphi_k^+] | 0\rangle = \delta(k - k') \langle 0 | 0\rangle = \delta(k - k').$$

Equalities of the form $H_0 \varphi_k^+ |0\rangle = E_0(k) \varphi_k^+ |0\rangle$ are easily checked using the commutation relations of the operators. Note that since the energy of V and N is independent of the momentum, the eigenstates of H_0 are the vectors $\int f_1(r) V^+(r) dr |0\rangle$, $\int f_2(r) N^+(r) dr\, |0\rangle$ with arbitrary functions $f_1(r)$ and $f_2(r)$. We will also require states in which two particles — N and θ — coexist. The corresponding vectors $N_{k_1}^+ \varphi_{k_2}^+ |0\rangle$ are normalized to δ-functions and

$$E = m_N + \mu + \frac{k_\theta^2}{2\mu}.$$

Switching on the interaction. We now add to the Hamiltonian an interaction term corresponding to the reaction $V \rightleftarrows N + \theta$, which has the

* The mass of a "bare" particle V, which is an eigenvalue of the Hamiltonian H_0 without interaction, is designated by m_0. The notation m_V is introduced at a later stage; it corresponds to the "physical" particle V.

form $V^+N\varphi + VN^+\varphi^+$. For simplicity we assume that all these operators are taken at the same point, so that

$$H_1 = g\int [V^+(r)\,N(r)\,\varphi(r) + V(r)\,N^+(r)\,\varphi^+(r)]\,dr. \tag{51.5}$$

Although in the nonrelativistic theory we can consider nonlocal interaction, i.e., "action at a distance", on passing to the relativistic case nonlocality in space inevitably leads to nonlocality in time and clashes with the causality principle. We will therefore consider local interaction only. In the momentum representation,

$$H_1 = g\Omega^{-1/2}\sum_{k_1,\,k_2,\,k_3}(V^+_{k_1}N_{k_2}\varphi_{k_3} + V_{k_1}N^+_{k_2}\varphi^+_{k_3})\,\delta_{k_1,\,k_2+k_3}, \tag{51.6}$$

where Ω is the volume where the particles are observed. Changing over from summation over $\boldsymbol{k}$ to integration over $\boldsymbol{k}$, we find

$$H_1 = \frac{g}{(2\pi)^{3/2}}\int d\boldsymbol{k}_1\,d\boldsymbol{k}_2\,d\boldsymbol{k}_3\,(V^+_{\boldsymbol{k}_1}N_{\boldsymbol{k}_2}\varphi_{\boldsymbol{k}_3} + V_{\boldsymbol{k}_1}N^+_{\boldsymbol{k}_2}\varphi^+_{\boldsymbol{k}_3})\,\delta(\boldsymbol{k}_1 - \boldsymbol{k}_2 - \boldsymbol{k}_3). \tag{51.6'}$$

It is readily seen that a system described by the total Hamiltonian

$$H = H_0 + H_1$$

has two simple conservation laws

$$\left.\begin{aligned} n_V + n_N &= n_1 = \text{const},\\ n_V + n_\theta &= n_2 = \text{const}, \end{aligned}\right\} \tag{51.7}$$

where n_V, n_N, and n_θ are the total numbers of V, N and θ particles. As the eigenstates of the system we therefore naturally choose states with definite values of these conserved numbers. As these numbers are always positive (no antiparticles), the corresponding functions contain a finite number of particles and the problem can be solved exactly (without using the perturbation theory, say).

It is readily seen that the free N and θ particles remain eigenstates even when the interaction is turned on, and the energy of these states does not change, i.e.,

$$\left.\begin{aligned} (H_0 + H_1)\,N^+_{\boldsymbol{k}}|0\rangle &= m_N N^+_{\boldsymbol{k}}|0\rangle,\\ (H_0 + H_1)\,\varphi^+_{\boldsymbol{k}}|0\rangle &= \left(\mu + \frac{\boldsymbol{k}^2}{2\mu}\right)\varphi^+_{\boldsymbol{k}}|0\rangle. \end{aligned}\right\} \tag{51.8}$$

However, a "bare" V particle — $V^+_{\boldsymbol{k}}|0\rangle$ — is no longer an eigenvector of the total Hamiltonian. The state of the physical V particle, $|V_{\text{phys},\,0}\rangle \equiv |V_0\rangle$, will first be solved in the first order of the perturbation theory. The matrix elements of the interaction Hamiltonian H_1 for transitions from the state $V^+_0|0\rangle$ do not vanish only for the states $N^+_{-\boldsymbol{k}}\varphi^+_{\boldsymbol{k}}|0\rangle$. We may therefore write

$$|V_{\text{phys},\,0}\rangle = |V_0\rangle = V^+_0|0\rangle + \int d\boldsymbol{k} f(\boldsymbol{k})\,N^+_{-\boldsymbol{k}}\varphi^+_{\boldsymbol{k}}|0\rangle, \tag{51.9}$$

where $f(k)$ is of first order in g. The coefficient before $V_0^+|0\rangle$ is taken equal to unity, since we are working in the first order of the perturbation theory.

We start with the equation

$$(H_0 + H_1)|V_0\rangle = m_V|V_0\rangle. \tag{51.10}$$

It is highly significant that already in the first order of the perturbation theory we use the exact energy m_V, which is shifted relative to m_0. Note that although the first-order correction to energy is zero, $m_0 - m_V$ is infinite already in the second order of the perturbation theory.

Equating the terms with $N_{-k}^+\varphi_k^+|0\rangle$, we find

$$f(k) = -\frac{g(2\pi)^{-3/2}}{E_N(k) + E_\theta(k) - m_V} = -\frac{g(2\pi)^{-3/2}}{m_N + \mu + \frac{k^2}{2\mu} - m_V}. \tag{51.11}$$

Thus the probability of finding a physical V particle in form N and θ with momenta between k and $k + dk$ is given in the first order of the perturbation theory by

$$\frac{g^2}{[E(k) - m_V]^2}\frac{dk}{(2\pi)^3}. \tag{51.12}$$

The exact solution hardly differs from the first order of the perturbation theory. Since the eigenstates of H constitute a complete system, we naturally seek an eigenvector of H as a superposition of the eigenvectors of H_0. Each term in this sum should correspond to the same "charge" values n_1 and n_2 as $V^+|0\rangle$ does: $n_1 = 1$, $n_2 = 1$. Apart from $V^+|0\rangle$, the only vectors meeting this requirement are the two-particle states $N_{k_1}^+\varphi_{k_2}^+|0\rangle$. The solution is therefore sought in the form

$$|V_0\rangle = Z^{\frac{1}{2}}\left[V_0^+|0\rangle + \int dk_1\, dk_2\, f(k_1, k_2)\, N_{k_1}^+\varphi_{k_2}^+|0\rangle\right]. \tag{51.13}$$

The meaning of this expression is quite obvious: the state of a physical V particle is sought as a "bare" V particle surrounded by a cloud of decay products (possibly virtual). The constant Z is introduced for normalization purposes; for simplicity we consider a V particle at rest. The next requirement is that $|V_0\rangle$ be an eigenvector of $H_0 + H_1$ corresponding to the eigenvalue m_V, which is the observable mass of the V particle. The momentum is automatically conserved:

$$f(k_1, k_2) = f(k_2)\,\delta(k_1 + k_2).$$

The equation therefore reduces to the form

$$(H_0 + H_1)\left[V_0^+ + \int dk\, f(k)\, N_{-k}^+\varphi_k^+\right]|0\rangle = m_V\left[V_0^+ + \int dk\, f(k)\, N_{-k}^+\varphi_k^+\right]|0\rangle.$$

Equating the coefficients of $N_{-k}^+\varphi_k^+|0\rangle$, we obtain for $f(k)$ the previous expression (51.11).

Let $\varkappa^2 = 2\mu (m_N + \mu - m_V) > 0$. This will make the V particle stable.* Further equating the terms with $V_0^+|0\rangle$, we find

$$m_0 = m_V - g(2\pi)^{-3/2}\int dk\, f(k) =$$

$$= m_V + g^2 \frac{1}{(2\pi)^3}\int \frac{dk}{E(k) - m_V} = m_V + \frac{\mu g^2}{\pi^2}\int_0^\infty \frac{k^2\, dk}{\varkappa^2 + k^2}. \qquad (51.14)$$

This equation can be considered as an expression for the observable mass m_V in terms of m_0 and g. However, m_V enters this expression in a fairly complex form, namely as a free term and through $\varkappa^2$. A better policy therefore is to determine m_0 in terms of g and the experimentally observed mass m_V. If the interaction is strictly local, i.e., of the form (51.5), the integral in (51.14) is divergent. Note that it also diverges when a relativistic dependence of E on k is assumed. Hence, the bare mass m_0 should be plus infinity if we are to obtain a finite observable mass m_V. This is what we call the renormalization of the mass of the V particle. Let us now compute the normalization constant Z taking $\langle V_{\text{phys}}|V_{\text{phys}}\rangle = 1$. We find

$$Z^{-1} = 1 + \frac{g^2}{(2\pi)^3}\int \frac{dk}{[E(k) - m_V]^2}. \qquad (51.15)$$

For nonrelativistic $E(k)$, this integral converges in a theory with scalar local interaction. However, if vector interaction is considered (see below), this integral is also divergent. For relativistic $E(k)$ the integral diverges for the scalar interaction as well.

Note another important equality:

$$Z^{-1} = \frac{dm_0}{dm_V}. \qquad (51.16)$$

It is applicable in the relativistic case too, when both Z^{-1} and m_0 are expressed by divergent integrals.

To understand the physical meaning of this equality, we apply to a system in the state $|V_0\rangle$ a small perturbation of the form $\Delta H = \Delta m_0 V_0^+ V_0$. The mass of the physical V particle changes, $\Delta m = B\Delta m_0$, where the coefficient B is the fraction of the "bare" V particle contained in the physical V particle, i.e., $B = Z$. Note that this method for determining the fraction of the "bare" V particle in the physical V particle is analogous to the magnetic-field timing device used in Chapter 5 for measuring particle collision times.

The exact probability of finding a physical V particle in the form θ and N is thus

$$\frac{g^2 Z}{[E(k) - m_V]^2}\frac{dk}{(2\pi)^3},$$

i.e., the g^2 of the perturbation-theoretical solution is replaced by g_r^2:

$$g_r^2 = Zg^2 = g^2\left\{1 + \frac{g^2}{(2\pi)^3}\int \frac{dk}{[E(k) - m_V]^2}\right\}^{-1} = g^2(1 + g^2 I_1)^{-1}. \qquad (51.17)$$

* For an unstable V particle $m_V = \mathrm{Re}\, m_V + i\,\mathrm{Im}\, m_V$; the integration contour over k should isolate outgoing waves only (see Chapter 5).

Since this probability is an observable, we actually observe the renormalized charge g_r^2. It is highly significant that g_r^2 enters the expression for the scattering cross section, which is clearly an observable.

Scattering in scalar interaction. When interaction is introduced in the Hamiltonian, the state with coexisting N and θ with definite momenta is no longer an eigenstate. In simple terms this means that scattering is observed. Consider the time-independent problem with scattering of θ by N.* We will work in the center-of-mass system (this is not essential, however, since N and V are much heavier than θ). As always, the solution includes the incident wave $N^+_{-k_0}\varphi^+_{k_0}|0\rangle$, the scattered wave, and the virtual V particle ("bare", not physical):

$$\Phi = N^+_{-k_0}\varphi^+_{k_0}|0\rangle + \int dk\, \chi(k)\, \varphi^+_k N^+_{-k}|0\rangle + CV^+_0|0\rangle, \tag{51.18}$$

and we further demand that

$$(H_0 + H_1)\,\Phi = E(k_0)\,\Phi, \tag{51.19}$$

where

$$E(k) = m_N + \mu + \frac{k^2}{2\mu}.$$

From (51.19) we obtain the set of equations

$$\left.\begin{aligned} \chi(k)\,[E(k) - E(k_0)] + g(2\pi)^{-3/2} C = 0,\ |k| \neq |k_0|, \\ C\,[m_0 - E(k_0)] + g(2\pi)^{-3/2}\Big[1 + \int dk\, \chi(k)\Big] = 0. \end{aligned}\right\} \tag{51.20}$$

The function $\chi(k)$ has a pole at $|k| = |k_0|$, $\chi(k) \approx \frac{B}{k^2 - k_0^2 - i\varepsilon}$. Its residue at this pole, as is readily seen, determines the scattering amplitude $A = 2\pi^2 B$ and hence the scattering cross section. For C we get

$$C\Big[E(k_0) - m_0 + \frac{g^2}{(2\pi)^3}\int \frac{dk}{E(k) - E(k_0) - i\varepsilon}\Big] = \frac{g}{(2\pi)^{3/2}}. \tag{51.21}$$

The integral in this expression is divergent and at a first glance it would therefore seem that we should take $C = 0$, $\chi = 0$, thus eliminating all scattering of θ by N in our model. Note, however, that we are dealing with a difference between a divergent integral and the infinite mass m_0. Carrying out mass renormalization and expressing m_0 in terms of the observable mass m_V and the (divergent) integral from (51.14), we obtain adding up two integrals a finite, convergent expression:

$$\begin{aligned} &-m_0 + \frac{g^2}{(2\pi)^3}\int \frac{dk}{E(k) - E(k_0) - i\varepsilon} = \\ &= -m_V - \frac{g^2}{(2\pi)^3}\int \frac{dk}{E(k) - m_V} + \frac{g^2}{(2\pi)^3}\int \frac{dk}{E(k) - E(k_0) - i\varepsilon} = \\ &= -m_V + \frac{g^2}{(2\pi)^3}\int \frac{(E(k_0) - m_V)\,dk}{(E(k) - E(k_0) - i\varepsilon)(E(k) - m_V)}, \\ &C\Big[E(k_0) - m_V + \frac{g^2}{(2\pi)^3}\int \frac{(E(k_0) - m_V)\,dk}{[E(k) - E(k_0) - i\varepsilon]\,[E(k) - m_V]}\Big] = \frac{g}{(2\pi)^{3/2}}. \end{aligned} \tag{51.22}$$

* A more difficult problem is that of scattering of θ by V, which was considered by Källen and Pauli /213/. The $\theta - V$ scattering amplitude was first determined by Amado /214/ and the wave functions of the particle were derived in a number of recent studies /215–219/.

To use more precise terms, we improved the convergence of the integral by adding another power $E(k) \sim k^2$ in the denominator following the elimination of m_0 from the original integral. In particular, this integral converges in our model and we say that mass renormalization is sufficient to eliminate the divergences. This, however, is not so for the relativistic $E(k)$. Therefore, in order to illustrate the various techniques for the elimination of divergences, we will carry out a further transformation so as to express the result in terms of the renormalized charge g_r^2. Let

$$I_2 = \frac{1}{(2\pi)^3}\int \frac{dk}{[E(k) - E(k_0) - i\varepsilon][E(k) - m_V]}. \tag{51.23}$$

For the scattered wave we have

$$\chi(k) = -\frac{1}{(2\pi)^3}\frac{1}{[E(k) - E(k_0)][E(k_0) - m_V]}\frac{g^2}{1 + g^2 I_2}. \tag{51.24}$$

Expressing g^2 in terms of g_r^2, we get

$$\chi(k) = -\frac{1}{(2\pi)^3}\frac{1}{[E(k) - E(k_0)][E(k_0) - m_V]}\frac{g_r^2}{1 + g_r^2(I_2 - I_1)},$$

where

$$I_2 - I_1 = \frac{E(k_0) - m_V}{(2\pi)^3}\int \frac{dk}{[E(k) - E(k_0) - i\varepsilon][E(k) - m_V]^2}. \tag{51.25}$$

Let us try to elucidate the logical aspects of renormalization, remembering that the actual interaction is not strictly local, being "fuzzed" over small distances $\sim \rho$, so that a cutoff is observed for extremely large momenta $\Lambda \sim \frac{1}{\rho}$. This indicates that the integration over dk does not extend to infinity but only to Λ.

For fixed Λ, all the expressions will be bounded. This does not mean, however, that they can be used conveniently, nor does it mean that we may take the limit as $\rho \to 0$ $(\Lambda \to \infty)$. This can be done only if the renormalized mass and charge m_V and g_r are known (and independent of Λ) and the results are expressed in terms of m_V and g_r. To illustrate this point, we list all the principal formulas in which we assume as given 1) m_0, g, Λ; 2) m_V, g, Λ; 3) m_V, g_r, Λ; $\Lambda \to \infty$.

$$1)\quad A = -\frac{\mu}{2\pi}\frac{g^2}{E(k_0) - m_0 + \frac{\mu g^2}{\pi^2}\left(\Lambda + \frac{\pi i}{2}k_0 - \frac{k_0^2}{\Lambda}\right)}, \tag{51.26}$$

$$m_0 = m_V + \frac{\mu g^2}{\pi^2}\left(\Lambda - \frac{\pi}{2}\varkappa + \frac{\varkappa^2}{\Lambda}\right),$$

$$g_r^2 = g^2\left[1 + \frac{\mu g^2}{\pi^2}\left(\frac{\pi}{2}\frac{\mu}{\varkappa} - \frac{2\mu}{\Lambda}\right)\right]^{-1};$$

$$2)\quad A = -\frac{\mu g^2}{2\pi}\frac{1}{E(k_0) - m_V}\frac{1}{1 + \frac{2\mu^2 g^2}{\pi^2}\left(\frac{\pi}{2}\frac{1}{\varkappa - ik_0} - \frac{1}{\Lambda}\right)}; \tag{51.26'}$$

$$3)\quad A = -\frac{\mu g_r^2}{2\pi}\frac{1}{E(k_0) - m_V}\frac{1}{1 + \frac{\mu^2 g_r^2}{2\pi\varkappa}\frac{\varkappa + ik_0}{\varkappa - ik_0}}. \tag{51.26''}$$

Note that on passing 1) → 2) → 3) the dependence of the scattering amplitude A on Λ for $\Lambda \to \infty$ is progressively weakened and in cases 2), 3) this amplitude has a finite limit for $\Lambda \to \infty$.

§ 52. THE COORDINATE REPRESENTATION

Very enlightening results are obtained when the problem of the physical V particle is solved directly in the coordinate representation /220/. As the Hamiltonian is invariant under Galilean transformations, the motion of the center of mass does not affect the final results. Therefore, as in all two-body problems of nonrelativistic quantum mechanics, we can eliminate this motion, and the problem thus reduces to the motion of a particle with reduced mass about an infinitely heave (fixed) center. In our case the reduced mass of N and θ, equal to $m_N\mu/(m_N+\mu)$, is nearly equal to the mass μ of the θ particle. We can therefore neglect the difference between these two masses, using μ throughout. Since the motion of the center of mass has been eliminated, we can introduce creation operators of V and N at one certain point (say, the origin), V^+ and N^+, such that $\langle 0|VV^+|0\rangle = 1$ and $\langle 0|NN^+|0\rangle = 1$. To obtain bounded results, we first take the Hamiltonian H_1 in which the interaction function is fuzzed over distances $\sim \rho$ (at a later stage we will pass to the limit as $\rho \to 0$). * This approach in fact corresponds to the renormalization technique. To simplify the calculations, we take the interaction function in the form $g(r) = g\frac{\delta(|r|-\rho)}{4\pi\rho^2}$ (so that $\int g(r)\,dr = g$). Then

$$H = H_0 + H_1 = m_0V^+V + m_NN^+N + \int \varphi^+(r)\left(\mu - \frac{1}{2\mu}\Delta\right)\times$$
$$\times\,\varphi(r)\,dr + \left[gV^+N\int\frac{\delta(|r|-\rho)}{4\pi\rho^2}\varphi(r)\,dr + \text{h.c.}\right]. \qquad (52.1)$$

The solution for the physical V particle is sought in the form

$$|V_{\text{phys}}\rangle = Z^{1/2}\left[V^+|0\rangle + N^+\int\psi(r)\,\varphi^+(r)\,dr\,|0\rangle\right]. \qquad (52.2)$$

The Sch. Eq. in this case gives

$$m_0 + g\psi(\rho) = m_V, \qquad (52.3)$$

$$\Delta\psi - \varkappa^2\psi = 2\mu g\frac{\delta(|r|-\rho)}{4\pi\rho^2} \qquad (52.4)$$

with $\varkappa^2 = 2\mu(m_N + \mu - m_V)$. (Here we made use of the spherical symmetry of $\psi(r)$.) If $\rho \ll 1/\varkappa$ (this can be always assumed, since $\rho \to 0$), equation (52.4) can be replaced** by

$$\Delta\psi - \varkappa^2\psi = 2\mu g\delta(r) \qquad (52.4')$$

* Strictly speaking, the following choice of $g(r)$ corresponds to interaction in a thin spherical shell of radius ρ.

** A more rigorous solution of equation (52.4) for $r \geqslant \rho$ differs from that of (52.4') by a term of second order of smallness in ρ. These corrections are ignored from the outset.

and then

$$\psi(r) = -2\mu g \frac{e^{-\varkappa r}}{4\pi r}, \tag{52.5}$$

$$m_0 = m_V + \frac{2\mu g^2}{4\pi} \frac{e^{-\varkappa\rho}}{\rho}. \tag{52.6}$$

Expanding (52.6) in powers of ρ and dropping all terms starting with the first order in ρ, we find

$$m_0 = m_V + \frac{\mu g^2}{2\pi} \frac{1}{\rho} - \frac{\mu g^2}{2\pi} \varkappa, \tag{52.6'}$$

whence we see that $m_0 \sim \frac{1}{\rho}$ for $\rho \to 0$. The wave function of the θ particle in the momentum representation ($f(k)$ in (51.11)) is readily seen to be the Fourier transform of $\psi(r)$ in (52.5). The normalization factor $Z = [1 + \int |\psi|^2 dr]^{-1}$ therefore coincides with the Z calculated in the momentum representation.

Expression (52.6') defines mass renormalization. We can also introduce renormalized charge $g_r^2 = Zg^2$. If we write

$$\int |\psi|^2 dr = \int dk\, |f(k)|^2 = g^2 I_1, \quad I_1 = \frac{\mu^2}{2\pi\varkappa}, \tag{52.7}$$

we find

$$Z^{-1} = 1 + g^2 I_1, \quad g^2 = \frac{g_r^2}{1 - g_r^2 I_1}. \tag{52.8}$$

It is clear from the last expression that the observable charge satisfies the inequality

$$g_r^2 \leqslant I_1^{-1} = \frac{2\pi\varkappa}{\mu^2}. \tag{52.9}$$

Otherwise $g^2 < 0$, i.e., g is imaginary. If g is imaginary, the Hamiltonian cannot be Hermitian, and this seriously clashes with the entire statistical interpretation of quantum mechanics. In particular, Z, which is equal to the probability of finding a physical V particle in the "bare" state $V^+|0\rangle$, becomes negative. Mass renormalization for $g^2 < 0$ leads to $m_V > m_0$. However, by the variational principle, an interaction which causes transformation between particles can only reduce the energy of the ground state. Thus, for $g^2 < 0$ we encounter nonphysical states of the V particle with $E < m_V$ (so-called "ghosts") /213/. Scattering of θ particles by physical V particles will involve transitions to "ghost" states, and at that with negative probabilities. All this renders the theory with $g_r^2 > g_c^2 = \frac{1}{I_1}$ unacceptable from physical standpoint.

Let us now consider the scattering problem. The solution of the Sch. Eq. $H\Phi = E\Phi$ with $E = m_N + \mu + \frac{k^2}{2\mu}$ is sought in the form

$$\Phi = CV^+|0\rangle + N^+ \int \psi_k(r)\, \varphi^+(r)\, dr\, |0\rangle, \tag{52.10}$$

where

$$\psi_k(r) = \frac{1}{2ikr}(-e^{-ikr} + S(k)\,e^{ikr}).$$

For $S(k)$ and C we obtain the equations

$$\left(\frac{k^2}{2\mu} + \mu + m_N - m_0\right)C = \frac{g}{2ik}\frac{S-1}{\rho} + \frac{g}{2}(S+1), \tag{52.11}$$

$$C = -\frac{\pi}{i\mu k g}(S-1). \tag{52.12}$$

Inserting for C in (52.11) its expression from (52.12) and m_0 from (52.6), we see that terms with $\frac{1}{\rho}$ cancel out. The theory is thus renormalizable, as for $\rho \to 0$, $m_0 \to \infty$, but the scattering results approach a limit which is independent of the cutoff radius.

The mass m_0 of the bare V particle also drops out from the equations and the final result contains $\varkappa$, which depends on the mass of the physical V particle.

After elementary algebraic manipulations, we find

$$ik\frac{1+S}{1-S} = \varkappa + \frac{\pi}{g^2\mu^2}(k^2 + \varkappa^2). \tag{52.13}$$

We can now easily find an expression for the scattering amplitude:

$$A = -\frac{\frac{\mu g^2}{2\pi}}{1 + \frac{\mu^2 g^2}{\pi}\frac{1}{\varkappa - ik}}\frac{1}{E+Q},\quad Q = m_N + \mu - m_V. \tag{52.14}$$

Note that fairly often the physical (renormalized) charge is defined by the pole term of the scattering amplitude:

$$A \sim -\frac{\mu g_r^2}{2\pi(E+Q)} \text{ for } E \to -Q. \tag{52.15}$$

Since the residue of the scattering amplitude at the pole $E = -Q$ is

$$\operatorname{Res} A = -\frac{\mu g^2}{2\pi\left(1 + \frac{\mu^2 g^2}{2\pi\varkappa}\right)}, \tag{52.16}$$

this definition is equivalent to the definition (51.17).

From (52.16) we see that the residue of the scattering amplitude is negative and its absolute value is bounded from above:

$$|\operatorname{Res} A|_{E=-Q} < \frac{\varkappa}{\mu},\quad \varkappa = \sqrt{2\mu Q}. \tag{52.17}$$

Note that this restriction on the residue coincides with the constraint which is obtained from (15.9) for $R = 0$. This is not surprising, since (52.17) can be derived (using the result of /221/) proceeding only from analyticity and unitarity properties, which hold true both for potential scattering and for the Lee model.

The scattering amplitude A as a function of the complex variable k has another pole at $k = -i\left(\varkappa + \frac{\mu^2 g^2}{\pi}\right)$. This pole, however, lies on the nonphysical sheet of the complex E plane.

The renormalized charge g_r satisfies inequality (52.9), and it reaches its extreme value as the "bare" constant g goes to infinity.

In this case the fraction of the bare V particle contained in the physical V particle goes to zero, and in the limit the physical V particle is entirely "made up" of $N + \theta$.* Thus, the limiting value of the residue corresponds to a transition to a compound model of the V particle, made up of locally coupled N and θ.

We see from (52.14) that in the limit as $g^2 \to \infty$ the results completely coincide with the results of the theory of scattering by a singular potential with a discrete level at $E = -Q$.

As the fraction of $N + \theta$ in the amplitude of the physical V particle approaches unity, we are drawing progressively closer to the limit; the fraction of the bare V particle correspondingly goes to zero. In fact, the bare V particle as such vanishes and its role is confined to a carrier of the local interaction which binds the N and the θ in the physical particle. We are near the limit if $g^2 \gg \frac{2\pi\varkappa}{\mu^2}$. Thus as we approach the pole and $\varkappa$ becomes smaller, the limiting relations characteristic of the compound model become applicable progressively earlier, for progressively smaller values of g.

In this section we followed the method of /220/. In conclusion note that inequality (52.9) was first derived in /121/. The equality sign corresponds to the case treated by Landau /222/. The inequality was also generalized to the relativistic case /223/.

§ 53. INTERACTION WITH UNSTABLE INTERMEDIATE PARTICLE**

We will now solve the equations for the case of an unstable intermediate particle. We again follow the method of /220/.

Suppose that the time-dependent Sch. Eq. has a solution which is an exponential function of time (i.e., $\sim e^{-iE_0 t}$ with complex E_0), whose spatial part, describing the particles A and B, contains only an outgoing wave, i.e., $\psi \sim e^{ik_0 r}/r$. In this case k_0 is also a complex number. For this time-dependent but nevertheless exponential solution we may also use equations of the form (52.3) and (52.4).

The general approach here is the same as for a stable V particle: the properties of the physical unstable state, i.e., E_0 and k_0, $E_0 = \frac{k_0^2}{2\mu} + \mu + m_N$, are assumed to be known, and the nonphysical bare mass m_0 is expressed in terms of the physical quantity E_0, the charge g, and the cutoff radius ρ.

* In the language of renormalization constants, this corresponds to Z going to zero. In the relativistic case $Z = 0$ may be regarded as the condition that a given particle is a compound particle.

** An unstable particle in the Lee model was considered in /224, 225/.

Then we turn to the scattering problem, i.e., a problem with arbitrary real positive k, with incoming and outgoing waves, and find the scattering amplitude. We use the expression for m_0 in terms of E_0, g, ρ; as before, the terms with $1/\rho$ cancel, i.e., the result has a definite limit as $\rho \to 0$, $m_0 \to \infty$.

Before going into the actual details, we should make two remarks. The result cannot be derived from the previous result for a stable particle by formally replacing $\varkappa$ with $-ik_0$, since the bare mass m_0, although a non-physical quantity containing a term $1/\rho$ ($m_0 \to \infty$ for $\rho \to 0$), should be real if the Hamiltonian is to be Hermitian and unitarity is to be observed. Formal substitution of $-ik_0$ for $\varkappa$ in (52.6') does not ensure a real m_0.

The second remark is purely technical: it is better to start with $k_0 = v - iw$ and express the final result in terms of v and w, which are both real and positive.

Thus for an unstable state

$$\psi(r) = C\frac{e^{ivr+wr}}{r}, \quad E_0 = \frac{v^2-w^2}{2\mu} - i\frac{vw}{2\mu} + \mu + m_N. \tag{53.1}$$

Inserting $\psi(r)$ in the Sch. Eq., we see that the terms $E_0\psi$ and $\left(\mu + m_N - \frac{\Delta}{2\mu}\right)\psi$ again cancel and as in (52.5) we obtain

$$\psi(r) = -\frac{\mu g}{2\pi}\frac{e^{ivr+wr}}{r}. \tag{53.2}$$

Insertion of (53.2) in (52.3) gives

$$m_0 = E_0 + \frac{\mu g^2}{2\pi}\left(\frac{1}{\rho} + w + iv\right) = \frac{v^2-w^2}{2\mu} - i\frac{vw}{\mu} + \frac{\mu g^2}{2\pi}\left(\frac{1}{\rho} + w + iv\right). \tag{53.3}$$

Unlike (52.6'), this is a complex equation. Since m_0 is real, the real part of (53.3) immediately gives

$$w = \frac{\mu^2 g^2}{2\pi}. \tag{53.4}$$

The problem with a stable V particle was characterized by two parameters, Q (or $\varkappa$) and g. The problem with an unstable particle is characterized by three parameters v, w, and g, but not all of them are independent: relation (53.4) leaves only two independent parameters. For the sake of simplicity, we henceforth express g^2 in terms of w.

In particular

$$m_0 = \frac{v^2+w^2}{2\mu} + \frac{w}{\mu}\frac{1}{\rho}. \tag{53.5}$$

Now consider the scattering problem. Equations (52.10)—(52.12) remain in force, the only difference being that we use (53.5) for m_0 and in the final result express g^2 in terms of w by (53.4). After simple algebraic manipulations, we obtain

$$ik\frac{1+S}{1-S} = \frac{k^2-v^2-w^2}{2w}, \tag{53.6}$$

$$S = \frac{(k-v-iw)(k+v-iw)}{(k-v+iw)(k+v+iw)}. \tag{53.7}$$

The function S (and hence the scattering amplitude) has two poles in the lower k halfplane at $k = \pm v - iw$. In the upper k halfplane, i.e., on the first E sheet, there are no poles.

Clearly for $\psi(r)$ of the form (53.1)

$$\frac{d \ln (r\psi)}{dr} = ik \frac{S+1}{S-1}. \tag{53.8}$$

Hence expression (53.8) for a stable particle gives in the limit as $g^2 \to \infty$

$$\frac{d \ln (r\psi)}{dr} = -\varkappa, \tag{53.9}$$

in accordance with the classical theory of Bethe and Peierls /20/. For an unstable V particle (53.6) gives

$$\frac{d \ln (r\psi)}{dr} = \frac{v^2}{2w} + \frac{w}{2} - \frac{k^2}{2w}, \tag{53.10}$$

which for real v and w and positive w can in no way be reduced to the form

$$\frac{d \ln (r\psi)}{dr} = \varkappa_1, \quad \varkappa_1 > 0, \tag{53.11}$$

corresponding to scattering by a singular potential with a virtual level (neutron—proton singlet interaction). In other words, calculations with an unstable particle give two poles in the k plane, which are arranged symmetrically about the imaginary axis in the lower halfplane.

A singular potential with a virtual level corresponds to a single pole on the imaginary axis in the lower halfplane, at $k = -i\varkappa_1$ (see (53.11)).

Even if we make the two poles of the unstable particle merge and move to the same point $k = -i\varkappa_1$, the result is a second-order pole, so that the equations will still be different from those in the case of a singular potential, when a first-order pole is involved.

In case of a stable particle, the two poles lie on the imaginary axis and do not coincide, so that one pole can be made to go to infinity, while the other remains fixed; in case of an unstable particle this cannot be accomplished, as the two poles are symmetric about the imaginary axis.

We see from (53.4) that in the limit as $g^2 \to \infty$, $w \to \infty$; insertion in (53.7) gives $S = 1$ for any finite k and v. Thus, the theory with an unstable particle has no meaningful limit in the case of strong coupling. This is the main distinction from the theory with a stable particle, which in the limit of strong coupling reduces to the deuton theory.

§ 54. INTERACTION BETWEEN N AND V

We will now consider the interaction of two heavy particles V and N.* We will show that, if the result is expressed in terms of the renormalized mass, it is free from divergent terms. Moreover, the renormalized charge will enter the result quite in a natural way.

* This problem was solved in the momentum representation in /226/.

A natural approach to this problem is in the adiabatic approximation. This means that first, making use of the smallness of the mass of the θ particle compared to m_V and m_N, we compute the wave function of θ for fixed N and V, separated by a distance b. The energy of this "state" depends on b as a parameter and can be considered as the potential energy of the interaction between V and N, associated with "emission" and "absorption" of θ particles. After that, we can easily solve the problem of motion of the particles V and N in this field (this will not be done here, however). Thus, the "state" of the particles V and N located at points $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ at a distance $b = |\boldsymbol{a}_1 - \boldsymbol{a}_2|$ from each other is described by the operators $V_1^+(N_1^+)$ and $V_2^+(N_2^+)$, namely the creation operators of $V(N)$ at points $\boldsymbol{r} = \boldsymbol{a}_1$ and $\boldsymbol{r} = \boldsymbol{a}_2$. The Hamiltonian $H = H_0 + H_1$ is written in the form

$$\left.\begin{aligned} H_0 &= m_0(V_1^+V_1 + V_2^+V_2) + m_N(N_1^+N_1 + N_2^+N_2) + \\ &\qquad + \int \varphi^+\left(\mu - \frac{1}{2\mu}\Delta\right)\varphi d\boldsymbol{r}, \\ H_1 &= g\left[V_1^+N_1\int\frac{\delta(|\boldsymbol{r}-\boldsymbol{a}_1|-\rho)}{4\pi\rho^2}\varphi(\boldsymbol{r})\,d\boldsymbol{r} + \right. \\ &\qquad \left. + V_2^+N_2\int\frac{\delta(|\boldsymbol{r}-\boldsymbol{a}_2|-\rho)}{4\pi\rho^2}\varphi(\boldsymbol{r})\,d\boldsymbol{r}\right] + \text{h. c.} \end{aligned}\right\} \tag{54.1}$$

The most general form of the physical state with one V particle and one N particle at a distance $\boldsymbol{b} = \boldsymbol{a}_1 - \boldsymbol{a}_2$ is

$$|VN\rangle = C_1V_1^+N_2^+|0\rangle + C_2V_2^+N_1^+|0\rangle + N_1^+N_2^+\int\psi(\boldsymbol{r})\varphi^+(\boldsymbol{r})\,d\boldsymbol{r}\,|0\rangle. \tag{54.2}$$

Since the Hamiltonian H is invariant under the transformation $1 \rightleftarrows 2$, the "eigenstates" can be classified according to the number $I = \pm 1$, where $C_2 = IC_1$. The energy E of such a "state" is written in the form

$$E = m_V + m_N + \varepsilon, \tag{54.3}$$

since it is clear from the start that for $b \to \infty$ we should have $E \to m_V + m_N$ (in this case $\varepsilon \to 0$). Solving the Sch. Eq., we obtain

$$\psi(\boldsymbol{r}) = -\frac{\mu g C_1}{2\pi}\left[\frac{e^{-\eta r_1}}{r_1} + I\frac{e^{-\eta r_2}}{r_2}\right], \tag{54.4}$$

$$(m_0 - m_V - \varepsilon)C_1 + g\psi|_{r_1=\rho} = 0, \tag{54.5}$$

where

$$r_1 = |\boldsymbol{r} - \boldsymbol{a}_1|,\ r_2 = |\boldsymbol{r} - \boldsymbol{a}_2|,$$
$$\eta^2 = 2\mu(m_N + \mu - m_V - \varepsilon) = \varkappa^2 - 2\mu\varepsilon.$$

Insertion of (54.4) in (54.5) gives

$$(m_0 - m_V - \varepsilon) = \frac{\mu g^2}{2\pi}\left[\frac{e^{-\eta r_1}}{r_1} + I\frac{e^{-\eta r_2}}{r_2}\right]_{r_1=\rho}, \tag{54.6}$$

or

$$\left(m_0 - m_V + \frac{\eta^2 - \varkappa^2}{2\mu}\right) = \frac{\mu g^2}{2\pi}\left[\frac{e^{-\eta r_1}}{r_1} + I\frac{e^{-\eta r_2}}{r_2}\right]_{r_1=\rho}. \tag{54.6'}$$

From this equation we can find η and thus ε.

We should now consider the limit as $\rho \to 0$. Expanding $\psi|_{r_1=\rho}$ in (54.6') in powers of ρ, we drop terms of first and higher orders; then

$$\left(m_0 - m_V + \frac{\eta^2 - \varkappa^2}{2\mu}\right) = \frac{\mu g^2}{2\pi}\left(\frac{1}{\rho} - \eta + I\frac{e^{-\eta b}}{b}\right). \tag{54.7}$$

For fixed m_0 and $\rho \to 0$, the result is unbounded.

It is at this stage that we apply mass renormalization (52.6'), whereby the mass m_V is expressed in terms of m_0 and $\frac{1}{\rho}$. Thus (54.7) takes the form

$$\left(\frac{g^2\mu}{2\pi}\frac{1}{\rho} - \frac{g^2\mu}{2\pi}\varkappa + \frac{\eta^2 - \varkappa^2}{2\mu}\right) = \frac{g^2\mu}{2\pi}\left[\frac{1}{\rho} - \eta + I\frac{e^{-\eta b}}{b}\right].$$

The terms with $\frac{1}{\rho}$ cancel and we can let ρ go to zero. We thus obtain the equation

$$\frac{\eta^2 - \varkappa^2}{2\mu} = \frac{\mu}{2\pi} I g^2 \left[1 + g^2 \frac{\mu^2}{\pi(\eta + \varkappa)}\right]^{-1} \frac{e^{-\eta b}}{b}. \tag{54.8}$$

If g is replaced by its expression in terms of g_r,

$$g^2 = g_r^2\left[1 - g_r^2 \frac{\mu^2}{2\pi\varkappa}\right]^{-1},$$

the equation takes the form

$$-\varepsilon = \frac{\eta^2 - \varkappa^2}{2\mu} = I\frac{\mu}{2\pi} g_r^2 \left[1 - g_r^2 \frac{\mu^2(\eta - \varkappa)}{2\pi\varkappa(\eta + \varkappa)}\right]^{-1} \frac{e^{-\eta b}}{b}. \tag{54.8'}$$

Equations (54.8) or (54.8') determine the energy of the (VN) system for fixed b. We see that for $I = +1$ the particles V and N are attracted, $E - (m_V + m_N) = \varepsilon = \frac{\varkappa^2 - \eta^2}{2\mu} < 0$, and for $I = -1$ they are repelled.

For $b \gg \varkappa$, $\varepsilon(b)$ is approximately the Yukawa potential

$$\varepsilon = -I\frac{\mu}{2\pi} g_r^2 \frac{e^{-\varkappa b}}{b}. \tag{54.9}$$

Thus, the interaction potential between N and V, $U(b) \equiv \varepsilon(b)$, depends on whether the particles N and V are in symmetric (in particular, s-wave) or in antisymmetric (in particular, p-wave) state. This is not surprising, since the interaction associated with exchange of θ particles gives rise both to ordinary and exchange forces. Note that the presence of two different potentials does not spoil the orthogonality of the wave functions, since wave functions which are solutions of the Sch. Eq. with different $U(r)$ have different symmetry and are thus automatically orthogonal to one another.

§ 55. VECTOR INTERACTION

Let the fermions V and N have spin 1/2 and the bosons θ have spin 0. The wave functions of V and N additionally depend on a spin variable. For $s = 1/2$ we are dealing with two-component wave functions. In accordance

with the usual convention of specifying spin functions, we assume that the first component corresponds to the state $s_z = +1/2$ and the second component to $s_z = -1/2$. These components will be subscripted with a and b. We introduce corresponding creation operators for particles with upward and downward spins:

$$N_a^+, V_a^+ - s_z = +\frac{1}{2}; \quad N_b^+, V_b^+ - s_z = -\frac{1}{2}.$$

The density of the interaction Hamiltonian h corresponding to the reaction $V \rightleftarrows N\theta$ is a scalar which can be formed from the product of a spinor N, an Hermitian conjugate spinor V^+, and a scalar φ. One possible approach is to form a sum of products of corresponding components of N and V^+ (we know that such a sum is a scalar) and to multiply it by φ:

$$\mathrm{h}_1 = g\,(V_a^+ N_a + V_b^+ N_b)\,\varphi + \mathrm{h.c.} \tag{55.1}$$

This interaction in no way differs from the scalar interaction that we have so far dealt with. Indeed, if initially all the particles had their spins pointing up, the spin will remain up. Particles with antiparallel spins do not interact; the spin and the orbital momentum are separately conserved.

Another possible approach to this interaction, which should be independent of the momenta of V and N (i.e., independent of the space derivatives of $V(r)$ and $N(r)$) is the following: we act on the spinor N with the spin vector $\boldsymbol{s} = \frac{\boldsymbol{\sigma}}{2}$ and multiply the resulting spinor by the Hermitian conjugate spinor V^+. The result $V^+\boldsymbol{s}N$ is a vector, and therefore to obtain the scalar Hamiltonian density, it should be dot-multiplied by the vector $\nabla\varphi$. Let us write out in more detail the expression for $V^+\boldsymbol{s}N\nabla\varphi$, using the symbol h_2 for this scalar quantity. We have

$$\boldsymbol{s}\boldsymbol{\sigma} = \frac{1}{2}\begin{pmatrix} a_z & a_x - ia_y \\ a_x + ia_y & -a_z \end{pmatrix},$$

$$\mathrm{h}_2 = V^+\boldsymbol{s}N\nabla\varphi = \frac{1}{2}\left[V_a^+ N_a \frac{\partial}{\partial z} + V_a^+ N_b\left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right) + V_b^+ N_a\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right) - V_b^+ N_b \frac{\partial}{\partial z}\right]\varphi(r). \tag{55.2}$$

The interaction Hamiltonian is obtained in the following way: h_2 is multiplied by the interaction constant f, the Hermitian conjugate of the product is added, and the sum is integrated over the entire volume:

$$H_2 = \int [f\mathrm{h}_2(r) + \mathrm{h.c.}]\,dr. \tag{55.3}$$

For this Hamiltonian to be invariant under space inversion, i.e., to conserve parity, the product of the three wave functions $\psi_V^*\psi_N\psi_\theta$ should be a pseudoscalar, since $\boldsymbol{s}\nabla$ is a pseudoscalar operator (this follows from the fact that the spin $\boldsymbol{s}$ is a pseudovector). For this to be so, it is sufficient, say, if ψ_θ is a pseudoscalar, and ψ_V and ψ_N are real (not pseudo) spinors. Note, however, that if the Lee model corresponded to experimentally observed facts, we could in no way determine separately the individual parities of V, N, and θ from simple observation of reactions described by the Hamiltonians H_1 and H_2. From these observations we can only determine the product of

their parities (+1 for H_1 and −1 for H_2), since by conservation of n_1 and n_2 in any reaction, one V particle on one side of the "equality" invariably corresponds to one N and one θ on the other side. Similarly, we cannot establish the absolute parity of a proton (or a neutron), where "absolute parity" is defined assigning positive parity for the vacuum. This is so because in all nucleon reactions the baryon charge is conserved, and we can only determine the product of the individual parities of the particles taking part in the reaction. On the other hand, the parity of the π^0 meson (equal to −1) can be determined in absolute terms, since the exact conservation laws do not forbid a reaction of the type $N \to N + \pi^0$ (here N is a nucleon). In the particular case of the π^0 meson the parity can also be found from its decay into two γ quanta. In these reactions the parity of the π^0 meson is inferred from the polarization ratio of the two γ quanta, irrespective of the parity assigned to the electromagnetic field (the parity of a system of two γ quanta with zero resultant momentum is +1 for parallel polarizations and −1 for antiparallel polarizations). The parity of π^+ and π^- mesons is taken equal to the parity of the π^0 meson (i.e., negative), since these three particles constitute an isotopic multiplet.

In summing, we can say that the determination of the absolute (i.e., relative to the vacuum) parity is feasible only for particles whose conserved quantum numbers are the same as those of the vacuum (π^0 falls in this category) and moreover only when the particle decay is governed by parity-conserving interaction.

To return to the vector interaction, we write H_2 in the momentum representation, dropping the subscript $\boldsymbol{k}$ of V and N and omitting the factor $\delta(\boldsymbol{k}_1 - \boldsymbol{k}_2 - \boldsymbol{k}_3)$, which accounts for momentum conservation:

$$\left.\begin{aligned} H_2 &= (2\pi)^{-3/2}\int d\boldsymbol{k}\,[ifV^+(s\boldsymbol{k})\,N\varphi_{\boldsymbol{k}} + \text{h. c.}\,], \\ \boldsymbol{k} &= \{k\sin\theta\cos\varphi,\ k\sin\theta\sin\varphi,\ k\cos\theta\}, \\ ifV^+(s\boldsymbol{k})\,N\varphi_{\boldsymbol{k}} &= if\frac{k}{2}\,(V_a^+N_a\cos\theta + V_a^+N_b\sin\theta e^{-i\varphi} + \\ &\quad + V_b^+N_a\sin\theta e^{i\varphi} - V_b^+N_b\cos\theta)\,\varphi_{\boldsymbol{k}}. \end{aligned}\right\} \tag{55.4}$$

As in the scalar case, the states of free motion of the θ particles $\varphi_{\boldsymbol{k}}^+|0\rangle$ and the N particle $(c_1N_a^+ + c_2N_b^+)|0\rangle$ are eigenstates of the total Hamiltonian $H_0 + H_2$. The state of the physical V particle (with its spin pointing up, say) is sought as a superposition of a "bare" V particle with its spin up and a cloud of N and θ:

$$|V_a\rangle = Z^{1/2}\Big\{V_a^+|0\rangle + \int d\boldsymbol{k}\,[\psi_a(\boldsymbol{k})\,N_a^+ + \psi_b(\boldsymbol{k})\,N_b^+]\,\varphi_{\boldsymbol{k}}^+|0\rangle\Big\}. \tag{55.5}$$

As in the case of scalar interaction, we first compute $\psi_a(\boldsymbol{k})$ and $\psi_b(\boldsymbol{k})$ to first order of the perturbation theory, with the same restrictions on m_0 and m_V. We find

$$\left.\begin{aligned} \psi_a(\boldsymbol{k}) &= \frac{1}{(2\pi)^{3/2}}\frac{k}{2}\frac{if\cos\theta}{E(k) - m_V} = \\ &= -\frac{k}{(2\pi)^{3/2}}\frac{if\sqrt{\pi}}{E(k) - m_V}\Big[-\sqrt{\frac{1}{3}}\,Y_{1,0}(\theta,\varphi)\Big], \\ \psi_b(\boldsymbol{k}) &= \frac{1}{(2\pi)^{3/2}}\frac{k}{2}\frac{if\sin\theta e^{i\varphi}}{E(k) - m_V} = \\ &= \frac{k}{(2\pi)^{3/2}}\frac{if\sqrt{\pi}}{E(k) - m_V}\Big[+\sqrt{\frac{2}{3}}\,Y_{1,+1}(\theta,\varphi)\Big], \end{aligned}\right\} \tag{55.6}$$

where

$$E(k) = m_N + \mu + k^2/2\mu.$$

The factors $\cos\theta$ and $\sin\theta e^{i\varphi}$ ensure momentum conservation: a V particle with spin up decays into an N particle with spin up and a θ particle with $l = 1$, $m = 0$, or an N particle with spin down and a θ particle with $l = 1$, $m = +1$. The conservation of j_z was clear from the start, since the Hamiltonian is invariant under rotations. The conversion of V_a^+ into N_a and θ with $l = 0$ is forbidden since the parity P of this state, equal to the product of the parity P_l of the coordinate function of θ ($P_l = (-1)^l$) and the internal parity $P_\theta = -1$, is negative for $l = 0$, whereas the parity of the V particle is $+1$. Thus, part of the time the V particle spends as N and θ in the p-state ($l = 1$). Clearly both terms in (55.6) correspond to the same value of j^3 and since for $V_a^+|0\rangle$, $j = \frac{1}{2}$, we should assign $j = \frac{1}{2}$ to the entire state. This can also be concluded from the Clebsch—Gordan coefficients, which are $+\sqrt{\frac{2}{3}}$ and $-\sqrt{\frac{1}{3}}$. Thus, during the fraction of the time when the physical V particle consists of N and θ, the orbital motion of θ corresponds to the state $p_{1/2}$ of the (N, θ) system.

Note that the cloud of θ around N in the $p_{1/2}$ state is spherically symmetric (if we sum over the two spin states of the N particle). Therefore, if θ is electrically charged, the V particle acquires no electric dipole moment, even though we are dealing with vector interaction. This is a direct consequence of parity conservation: the relation between the polar vector of the dipole electric moment and the axial spin vector cannot be invariant under space inversion.

In case of an unstable V particle the wave functions $\psi_a(k, \theta, \varphi)$ and $\psi_b(k, \theta, \varphi)$ characterize the angular distribution of the emitted decay products, N and θ. The distribution of the emitted θ particles is again spherically symmetric. Note, however, that for N particles emitted at a certain angle (the N particles are emitted in the opposite direction relative to the θ particles) we know not only the probability ratio of the states with $s_z = +1/2$ and $s_z = -1/2$, but also the phases of the corresponding amplitudes. This means that the N particles emitted at a certain angle (θ_N, φ_N) when polarized V particles decay (in our example $s_{zV} = +1/2$) are completely polarized. This is a much stronger proposition than that concerning the probability ratio for $s_{zN} = \pm 1/2$. The direction of the spin of the N particle will be defined as that direction along which the projection of its spin is $+1/2$ with sufficient likelihood; this direction will be specified by the polar angles Θ, Φ. The spin part of the wave function of this state is proportional to

$$\begin{pmatrix} \cos\frac{\Theta}{2} \\ \sin\frac{\Theta}{2} e^{i\Phi} \end{pmatrix}. \tag{55.7}$$

Comparing this expression with ψ_a and ψ_b we find

$$\Phi = \varphi_N, \quad \Theta = 2\theta_N. \tag{55.8}$$

That the particular Hamiltonian H_2 corresponds to interaction with the $p_{1/2}$ wave only is directly evident from the form of the Hamiltonian. To elucidate this point, we introduce the operators

$$\left.\begin{aligned}\varphi_{k,l,m} &= \frac{k}{(2\pi)^{3/2}}\int Y^*_{l,m}(\theta_k,\varphi_k)\,\varphi_k\,d\Omega_k,\\ \varphi_k &= \frac{(2\pi)^{3/2}}{k}\sum_{l,m}\varphi_{k,l,m}Y_{l,m}(\theta_k,\varphi_k),\end{aligned}\right\} \tag{55.9}$$

which destroy a free-moving θ particle with definite values of l and $l_z = m$; their Hermitian conjugates are the creation operators. Here $Y_{l,m}(\theta,\varphi)$ are normalized spherical functions.*

Inserting expression (55.9) for φ_k in (55.4) and integrating over $d\Omega_k$ we obtain

$$H_2 = (2\pi)^{-3/2}\int k\,dk\left\{if\sqrt{4\pi}\left[V_a^+\left(\sqrt{\tfrac{1}{3}}N_a\varphi_{k,1,0} - \right.\right.\right.$$

$$\left.\left.\left. - \sqrt{\tfrac{2}{3}}N_b\varphi_{k,1,+1}\right) + V_b^+\left(\sqrt{\tfrac{2}{3}}N_a\varphi_{k,1,-1} - \sqrt{\tfrac{1}{3}}N_b\varphi_{k,1,0}\right)\right] + \text{h.c.}\right\}. \tag{55.10}$$

If we now use the Clebsch—Gordan coefficients (see, e.g., /8/, where the normalization of $Y_{l,m}(\theta,\varphi)$ is also discussed) to introduce the destruction (creation) operators of an $N+\theta$ pair with definite values of l, j, and j_z,

$$\left.\begin{aligned}(N\theta)_n^{l+1/2,\,l} &= C_{11}^n\varphi_{k,l,n-1/2}N_a + C_{21}^n\varphi_{k,l,n+1/2}N_b,\\ (N\theta)_n^{l-1/2,\,l} &= C_{12}^n\varphi_{k,l,n-1/2}N_a + C_{22}^n\varphi_{k,l,n+1/2}N_b,\end{aligned}\right\} \tag{55.11}$$

H_2 is written in the form

$$H_2 = -(2\pi)^{-3/2}\int k\,dk\left\{if\sqrt{4\pi}\left[V_a^+(N\theta)_{1/2}^{1/2,\,1} + V_b^+(N\theta)_{-1/2}^{1/2,\,1}\right] + \text{h.c.}\right\}. \tag{55.12}$$

This means that V interacts only with the $p_{1/2}$ wave, i.e., the wave with $l = 1$, $j = 1/2$.

As in the scalar case, the exact solution differs from the first order of the perturbation theory only by a normalization factor $Z^{1/2}$. We have the equations

$$m_0 = m_V + \frac{|f|^2}{(2\pi)^3}\int_0^\infty \frac{k^2}{4}\frac{4\pi k^2\,dk}{E(k)-m_V}, \tag{55.13}$$

$$Z^{-1} = 1 + \frac{|f|^2}{(2\pi)^3}\int_0^\infty \frac{k^2}{4}\frac{4\pi k^2\,dk}{[E(k)-m_V]^2}. \tag{55.14}$$

In this case, the two integrals diverge. The reason for the divergence of the integral for Z^{-1} is very clear in the coordinate representation. While the s-wave solution near the origin behaves as r^{-1} and therefore $\int dr 4\pi r^2|\psi|^2$ converges, the p-wave solution near $r = 0$ behaves mainly as r^{-2} and it cannot be normalized on account of the excessive density of θ particles for small r. It also becomes clear why the "fuzzing" of the interaction over

* Note that the vectors $\varphi^+_{k,l,m}|0\rangle$ are normalized by the following relation:

$$\langle 0|\varphi_{k',l',m'}\varphi^+_{k,l,m}|0\rangle = \frac{1}{(2\pi)^3}\delta(k-k')\delta_{ll'}\delta_{mm'}.$$

a range $\sim\rho$ leads to convergence of the integrals and we see how the integrals depend on ρ. We now introduce the renormalized charge $|f_r|^2 = Z|f|^2$. The density of the θ cloud at a finite distance is proportional to $|f_r|^2$. It is thus $|f_r|^2$ which should be an observable.

The fundamental difference between this case and the scalar interaction is that here, already for an arbitrarily small $|f_r|^2 \neq 0$, we obtain

$$|f|^2 = \frac{|f_r|^2}{1-|f_r|^2 I_1} = -\infty^{-1} = 0,$$

since $I_1 = +\infty$. This means that for any $f_r \neq 0$ the system Hamiltonian is non-Hermitian, with all the ensuing unpleasantness. So as to avoid contradictions with the fundamental principles of quantum mechanics, the Hamiltonian must be kept Hermitian, and this requires cutoff at high momenta $\Lambda \sim \frac{1}{\rho}$. The following equality should thus be satisfied:

$$\frac{1}{(2\pi)^3}\int_0^{\Lambda} \frac{k^2}{4}\frac{4\pi k^2\,dk}{[E(k)-m_V]^2} \leqslant \frac{1}{|f_r|^2}. \tag{55.15}$$

Hence it is clear that as $|f_r|^2$ decreases, the maximum permissible Λ increases and the interaction approaches with better precision the local point interaction. For example, in quantum electrodynamics (where the formulas are naturally different from (55.15)) this condition takes the form

$$\Lambda \lessapprox m_e c \cdot e^{137}, \tag{55.16}$$

so that hopefully we are very far from that limit where a substantial modification of the theory will be required to fit the observed data. Hence it also follows that breakdown of quantum electrodynamics at energies much less than Λc would indicate substantial nonlocality of the theory. However, for $\Lambda \to \infty$ we should have $|f_r|^2 \to 0$. In the relativistic theory of elementary particles, an analog of this is the theorem of the "Moscow zero" /227/ which states that for $\Lambda \to \infty$ the observable interaction vanishes (if only Hermitian Hamiltonians are considered).

Scattering in the vector interaction. Scattering by vector interaction differs from the case of scalar interaction in that charge renormalization is essential if we are to obtain bounded results. Consider the scattering of a θ particle with initial momentum $\boldsymbol{k}_0 = (0, 0, k_0)$ by a polarized N particle with spin pointing up (treatment of the general case need not introduce any fundamental difficulties).

The solution of the equation

$$H|A\rangle = E(k_0)|A\rangle \tag{55.17}$$

is sought in the usual form

$$|A\rangle = N_a^+ \varphi_{k_0}^+|0\rangle + \int d\boldsymbol{k}\,[\chi_a(\boldsymbol{k})N_a^+ + \chi_b(\boldsymbol{k})N_b^+]\varphi_k^+|0\rangle + CV_a^+|0\rangle. \tag{55.18}$$

The term $V_b^+|0\rangle$ can be omitted from the outset, since the incident wave contains only states with $j_z = +1/2$. We thus obtain the equations

$$\left.\begin{aligned} C[m_0 - E(k_0) - i\varepsilon] &= -(2\pi)^{-3/2} if\left\{\frac{k_0}{2} + \int dk \frac{k}{2}[\chi_a(k)\cos\theta + \chi_b(k)\sin\theta e^{-i\varphi}]\right\}, \\ [E(k) - E(k_0) - i\varepsilon]\chi_a(k) &= \frac{k}{2}(2\pi)^{-3/2} if C\cos\theta, \\ [E(k) - E(k_0) - i\varepsilon]\chi_b(k) &= \frac{k}{2}(2\pi)^{-3/2} if C\sin\theta e^{i\varphi}. \end{aligned}\right\} \quad (55.19)$$

Solving these equations, we find χ_a and C (the expression for χ_b is entirely analogous):

$$\chi_a(k) = C\frac{k}{2}\frac{(2\pi)^{-3/2} if\cos\theta}{E(k) - E(k_0) - i\varepsilon}, \quad (55.20)$$

$$C = -(2\pi)^{-3/2} if\frac{k_0}{2}\cdot\left[m_0 - E(k_0) - \frac{|f|^2}{(2\pi)^3}\int_0^\infty \frac{k^2}{4}\frac{4\pi k^2\,dk}{E(k) - E(k_0) - i\varepsilon}\right]^{-1}. \quad (55.21)$$

Inserting for m_0 in (55.20) and (55.21) its expression in terms of the renormalized mass m_V and a divergent integral, we obtain

$$\chi_a = -\frac{k_0 k\cos\theta}{4}\frac{1}{(2\pi)^3}\frac{[E(k_0) - m_V]^{-1}}{E(k) - E(k_0) - i\varepsilon}\frac{|f|^2}{1 + |f|^2 I_2}. \quad (55.22)$$

Here the integral

$$I_2 = \frac{1}{(2\pi)^3}\int_0^\infty \frac{k^2}{4}\frac{4\pi k^2\,dk}{[E(k) - m_V][E(k) - E(k_0) - i\varepsilon]} \quad (55.23)$$

still diverges for large k, although less so than the integral in (55.15). Inserting the renormalized charge, we ensure convergence of the integral

$$I_3 = I_2 - I_1 = [E(k_0) - m_V]\frac{1}{(2\pi)^3}\int_0^\infty \frac{k^2}{4}\frac{4\pi k^2\,dk}{[E(k) - m_V][E(k) - E(k_0) - i\varepsilon]}, \quad (55.24)$$

and finally the scattering amplitude in the coordinate representation (see (21.5)—(21.9)) takes the form

$$\left.\begin{aligned} A_a(\theta,\varphi) &= -\frac{k_0^2\mu^2\cos\theta}{4\pi(\varkappa^2 + k_0^2)}\frac{|f_r|^2}{1 + |f_r|^2 I_3}, \\ A_b(\theta,\varphi) &= -\frac{k_0^2\mu^2\sin\theta e^{i\varphi}}{4\pi(\varkappa^2 + k_0^2)}\frac{|f_r|^2}{1 + |f_r|^2 I_3}, \\ I_3 &= \frac{\mu^4}{\pi}\frac{2\varkappa^3 - 3\varkappa(k_0^2 + \varkappa^2) - 2ik_0^2}{k_0^2 + \varkappa^2}. \end{aligned}\right\} \quad (55.25)$$

The differential scattering cross section $\frac{d\sigma}{d\Omega} = (|A_a|^2 + |A_b|^2)$ is seen to be independent of the scattering angle.

Note that although cutoff of large momenta is inevitable if we are to retain a Hermitian Hamiltonian, the amplitudes (55.25) are the limits as $\Lambda \to \infty$ of the amplitudes in the theory with cutoff. It is because we use renormalized mass and charge that the dependence of the amplitudes on Λ is such that the limit as $\Lambda \to \infty$ can be taken. Particular calculations are of course best carried out directly for the limit values.

Our model can be conveniently applied to the analysis of the polarization of scattered particles.

We start with a scalar interaction. In this case, as we have noted before, the initial polarization of the colliding particles (e.g., a certain spin orientation) is conserved after the collision, since the scalar interaction is spin independent. Therefore, if the N particles in the target are unpolarized, the scattered N particles will also be unpolarized. If the spins of the target N particles point in the direction of motion, the scattered N particles also have their spins in the primary direction, i.e., although scattering in this case does not produce polarization, the angle between the spin and the direction of motion is changed.

In the case of vector interaction, scattering in our model can be treated as formation of a V particle — the collision product of N and θ — which eventually decays into its constituents. Since the incident θ wave (it is taken to propagate in the direction of the z axis) contains only states with $m = 0$, V particles in states a and b are created with amplitudes which are proportional to the amplitudes of N in states a and b, respectively. After that the V particles decay. Since a bare V particle interacts only with the $p_{1/2}$ wave of N, θ, we conclude that the θ particles are scattered isotropically (as viewed in the center of mass system, of course) irrespective of the actual character and degree of polarization of the primary N. The magnitude of the scattering cross section is thus independent of polarization. Indeed, to any "pure", i.e., completely polarized, state of a created V particle we can assign a definite spin direction. Such a V particle, as we have seen before, decays and produces an isotropic distribution of θ particles. If the N target is partially polarized, so that it is described by a density matrix (in spin variables) and not by a wave function, the intermediate V particles are also described by a density matrix. Since the introduction of a density matrix is a way of averaging over an ensemble of "pure" noninteracting systems, the isotropy of scattering is not broken.

If the N target is initially unpolarized, the scattered N particles remain unpolarized in the vector case as well. This can be proved as follows. When a state $V_a^+|0\rangle$ decays, the N particles emitted at an angle (θ, φ) have their spins pointing in the direction (55.8); when $V_b^+|0\rangle$ decays the spins of the N particles emitted at the same angle point in the opposite direction. Thus, if the target is a mixture of $N_a^+|0\rangle$ and $N_b^+|0\rangle$ with uncorrelated phases, the states $V_a^+|0\rangle$ and $V_b^+|0\rangle$ and hence the scattered N particles will have uncorrelated phases, which proves that the scattered N particles are unpolarized. However, scattering by polarized N particles in case of vector interaction does not leave the direction of polarization unchanged.

§ 56. PARITY NONCONSERVATION IN THE LEE MODEL

The assumption of parity nonconservation in weak interaction led Lee and Yang /92/ to two fundamentally new conclusions concerning the behavior of elementary particles with spin.

The first conclusion related to the possibility of asymmetric, nonisotropic decay. The decay products should be preferably emitted in the direction of the momentum of the decaying particle (or in the opposite direction).

The other conclusion suggested the possible existence of a dipole moment in elementary particles, again parallel (or antiparallel) to the particle momentum.

The first of Lee and Yang's two conclusions was brilliantly confirmed in experiments with β decay of polarized nuclei /93/ and muons /228/. The predicted order of magnitude of the dipole moment, however, is definitely beyond the possibilities of experimental detection. Landau developed a comprehensive theory linking the nonconservation of parity in the decay of charged particles with space parity /299, 230/.*

Landau's theory retains invariance under time reversal ($t \to -t$), although the space parity is not conserved. Recent experimental results /94/ indicate that T-invariance is not exact either. However, the interaction breaking the T-invariance is apparently weaker than the interaction which changes the space parity.** Landau's theory with T-invariance is thus nevertheless of definite interest.

One of Landau's conclusions is that the dipole moment of elementary particles is identically zero. At a first glance it would appear that asymmetric decay should lead to a finite dipole moment: consider a polarized neutron with its momentum pointing up; it is an established fact that, when decaying, this neutron will emit electrons mostly up. Now consider the same polarized neutron in the spherically symmetric field of a nucleus; the energy relations are such that the neutron is stable, it does not decay. Virtual decay, however, is allowed and in fact inevitable: the neutron emits an electron, which is reabsorbed instantaneously; we may thus visualize the nucleus as surrounded by a cloud of virtual electrons.

Since the actual decay is asymmetric, the virtual decay can also be expected to show certain asymmetry, and an asymmetric cloud of virtual electrons should produce a dipole moment. Landau gave a general proof of the fallacy of this primitive reasoning. Ioffe /234/ established the dependence of decay asymmetry and dipole moment on the assumptions of T-invariance. The point is that the assumption of linear relation between the momentum $\boldsymbol{k}$ of the emitted particle and the direction of polarization (spin orientation) $\boldsymbol{s}$ of the decaying particle is consistent with time reversal: both vectors reverse their sign. The static dipole moment $\boldsymbol{d}$ or, alternatively, the static center of gravity of the cloud of virtual particles $\boldsymbol{r}$ do not change their sign when time is reversed. The spin $\boldsymbol{s}$ is therefore related to the static quantities $\boldsymbol{r}$ and $\boldsymbol{d}$ only in a theory which is not invariant under time reversal.

Consider the decay of V into N with the emission of θ, assuming a parity changing interaction in our model (V and N have spin 1/2). This will enable us to elucidate the dependence of the decay asymmetry of a polarized particle of spin 1/2 on the phases of the coupling constants in the expression for the decay interaction.

To first approximation, the decay asymmetry is found to depend on the imaginary part of the vector coupling constant, whereas the dipole moment depends on the real part of this constant, so that there is no direct relation between decay asymmetry and the dipole moment /208/.

* The possibility of combining mirror reflection with transformation to antiparticles was suggested independently by Lee and Yang.

** A detailed treatment of the properties of T-noninvariant interaction can be found in reviews /231, 232/. Note that the detection of the electric dipole moment of a particle (e.g., an electron or a nucleus) in a neutral atom is further complicated, as was observed by Schiff /233/, by the fact that screening suppresses the first order effects associated with the electric dipole moment.

We have already noted that for the total Hamiltonian to be invariant under space inversion, the product of the parities of V, N, and θ should be positive for scalar interaction (H_1) and negative for vector interaction (H_2). Hence it follows that a Hamiltonian which contains both H_1 and H_2 at the same time cannot be invariant under space inversion. Therefore prior to 1956 — before the discovery of parity changing interaction — considerations of invariance under space inversion automatically ruled out Hamiltonians with the sum $H_1 + H_2$. For parity changing weak interaction, however, we must consider Hamiltonians of the form $H_{\text{int}} = H_1 + H_2$.

Consider the decay $V \to N + \theta$. The problem will be considered in the first order of perturbation theory and the reverse process $\theta + N \to V$ is therefore ignored. Since we are not concerned with renormalization at this stage, no distinction is made between m_0 and m_V.

The coordinate representation is the most suitable for our purposes. First we isolate in explicit form the motion of the center of mass. The wave function of the V particle is taken in the form of a plane wave (the spin of V is assumed to point up):

$$|V\rangle = \int e^{ikr_1} V_a^+(r_1)\, dr_1 |0\rangle . \tag{56.1}$$

The operator $H_{\text{int}} = H_1 + H_2$ converts this state to a vector with N and θ:

$$|N,\theta\rangle = \sum_{i=a,b} \iint \psi_i(r_2, r_3)\, N_i^+(r_2)\, \varphi^+(r_3)\, dr_2 dr_3 |0\rangle \tag{56.2}$$

(i is the spin index of N).

The first-order perturbation equations have the usual form

$$H_{\text{int}}|V\rangle = [E_V(k) - H_0]|N\theta\rangle, \tag{56.3}$$

where H_0 is taken from (52.1) and $E_V(k) = m_V + k^2/2m_V$. We now write H_{int} in more detail:

$$H_{\text{int}} = \iiint \left\{ V_l(r_1) \left[g N_l^+(r_2) \varphi(r_3) + f \sigma_{lk} N_k^+(r_2) \frac{\partial}{\partial r_3} \varphi^+(r_3) \right] + \right. \\ \left. + \text{h.c.} \right\} \delta(r_1 - r_2)\, \delta(r_2 - r_3)\, dr_1\, dr_2\, dr_3. \tag{56.4}$$

The equations for $\psi_a(r_2, r_3)$, $\psi_b(r_2, r_3)$ are

$$\left.\begin{aligned} \left[E_V(k) - m_N - \mu + \frac{1}{2m_N}\Delta_{r_2} + \frac{1}{2\mu}\Delta_{r_3}\right]\psi_a(r_2, r_3) = \\ = e^{ikr_3}\left[g\delta(r_2 - r_3) + \frac{f}{2}\frac{\partial}{\partial z_3}\delta(r_2 - r_3)\right], \\ \left[E_V(k) - m_N - \mu + \frac{1}{2m_N}\Delta_{r_2} + \frac{1}{2\mu}\Delta_{r_3}\right]\psi_b(r_2, r_3) = \\ = e^{ikr_3}\frac{f}{2}\left(\frac{\partial}{\partial x_3} + i\frac{\partial}{\partial y_3}\right)\delta(r_2 - r_3). \end{aligned}\right\} \tag{56.5}$$

Making the standard substitution

$$R = \frac{m_N r_2 + \mu r_3}{\mu + m_N}; \quad r = r_3 - r_2,$$

we separate the variables

$$\psi_i(r_3, r_3) = e^{ikR}\psi_i(r);$$

for $\psi_i(r)$ we obtain an inhomogeneous Sch. Eq., with the mass μ replaced by the reduced mass of N and θ. Using the symbol μ to denote this reduced mass, we may write

$$\left.\begin{aligned}\Delta\psi_a + 2\mu E\psi_a &= 2\mu\left[g\delta(r) + \frac{f}{2}\frac{\partial}{\partial z}\delta(r)\right],\\ \Delta\psi_b + 2\mu E\psi_b &= 2\mu\frac{f}{2}\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)\delta(r).\end{aligned}\right\} \tag{56.6}$$

Here E is the energy released in the decay.

The decay is allowed for $E > 0$, when θ particles with momentum $p = \sqrt{2\mu E}$ are emitted. At large distances from the source, the solution should behave as an outgoing wave $\psi \sim e^{ipr}/r$. Indeed, in this case

$$\left.\begin{aligned}\psi_a &= -\frac{1}{4\pi}\left[g\frac{e^{ipr}}{r} + \frac{f}{2}\cos\theta\frac{d}{dr}\left(\frac{e^{ipr}}{r}\right)\right],\\ \psi_b &= -\frac{1}{4\pi}\frac{f}{2}e^{i\varphi}\sin\theta\frac{d}{dr}\left(\frac{e^{ipr}}{r}\right).\end{aligned}\right\} \tag{56.7}$$

For $pr \gg 1$,

$$\left.\begin{aligned}\psi_a &= -\frac{1}{4\pi}\frac{e^{ipr}}{r}\left[g + \frac{ipf}{2}\cos\theta\right],\\ \psi_b &= -\frac{1}{4\pi}\frac{e^{ipr}}{r}\frac{ipf}{2}e^{i\varphi}\sin\theta.\end{aligned}\right\} \tag{56.8}$$

For $E < 0$ real decay is forbidden. Virtual decay is described by a solution which falls off exponentially as $e^{-\varkappa r}/r$, where $\varkappa^2/2m = -E$. In this case we get

$$\left.\begin{aligned}\psi_a &= -\frac{1}{4\pi}\left[g\frac{e^{-\varkappa r}}{r} + \frac{f}{2}\cos\theta\frac{d}{dr}\left(\frac{e^{-\varkappa r}}{r}\right)\right] =\\ &= -\frac{1}{4\pi}\frac{e^{-\varkappa r}}{r}\left[g - \frac{f}{2}\varkappa\cos\theta\left(1 + \frac{1}{\varkappa r}\right)\right],\\ \psi_b &= -\frac{1}{4\pi}\frac{f}{2}e^{i\varphi}\sin\theta\frac{d}{dr}\left(\frac{e^{-\varkappa r}}{r}\right) =\\ &= \frac{1}{4\pi}\frac{f}{2}\frac{e^{-\varkappa r}}{r}e^{i\varphi}\sin\theta\left(1 + \frac{1}{\varkappa r}\right).\end{aligned}\right\} \tag{56.9}$$

These expressions provide an indication of decay asymmetry or of the asymmetry of the cloud of virtual particles when no actual decay takes place. A significant feature is the appearance of two terms in the expression for ψ_a: the transition of the V particle with $s_z = +1/2$ to N particle with $s_z = +1/2$ may be accompanied by emission of either an s-wave ($l = 0$) or a p-wave ($l = 1$, $m = 0$) θ particle. Interference of these two terms in ψ_a gives terms linear in cos θ which are associated with the spin orientation of the decaying V particle (θ is the angle between the direction of polarization of V (the z axis) and the radius-vector r).

The wave function ψ_b corresponds to a transition of V, $s_z = +1/2$ to N, $s_z = -1/2$. It describes a p-wave θ particle, $l = 1$, $m = +1$.

Since ψ_a and ψ_b are related to different orthogonal states of the N particle (spin up and spin down), there is no interference between ψ_a and ψ_b.

The current of θ particles for large r in the case $E > 0$ is

$$j = \frac{1}{2\mu i}(\psi_a^* \nabla \psi_a - \psi_a \nabla \psi_a^* + \psi_b^* \nabla \psi_b - \psi_b \nabla \psi_b^*) =$$
$$= \frac{1}{(4\pi)^2} \frac{k}{r^2 \mu} \frac{r}{r} \left[|g|^2 + \frac{k^2}{4} |f|^2 + \frac{ik}{2}(fg^* - f^* g) \cos\theta \right]. \qquad (56.10)$$

For $E < 0$, we are concerned only with the distribution of the density ρ of virtual θ particles, since the current at infinity is zero:

$$\rho = \psi_a^* \psi_a + \psi_b^* \psi_b = \frac{e^{-2\varkappa r}}{r^2} \frac{1}{(4\pi)^2} \left[|g|^2 + \frac{\varkappa^2}{4} |f|^2 \left(1 + \frac{1}{\varkappa r}\right)^2 - \right.$$
$$\left. - \frac{\varkappa}{2} \left(1 + \frac{1}{\varkappa r}\right)(fg^* + f^* g) \cos\theta \right]. \qquad (56.11)$$

Expressions (56.10) and (56.11) contain a highly significant result; they show that there is no identical relation between decay asymmetry and the asymmetry of the cloud of virtual particles: one depends on $g^* f - g f^*$ and the other on $g^* f + g f^*$.

Let the scalar coupling constant g be real (this can always be accomplished by a suitable gauge transformation).

It is readily seen that time reversal operation T reduces the Hamiltonian

$$H_1 = \int d\boldsymbol{k}\, i f V^+(\sigma \boldsymbol{k})\, N \varphi_{\boldsymbol{k}} + \text{h.c.} \qquad (56.12)$$

to the form

$$T^{-1} H_1 T = -\int d\boldsymbol{k}\, i f^* V^+(\sigma \boldsymbol{k})\, N \varphi_{\boldsymbol{k}} + \text{h.c.}, \qquad (56.12')$$

since this operation reverses the sign of the momentum $\boldsymbol{k}$ and the spin σ simultaneously and the c-numbers are replaced by their complex conjugates (the operator T is antiunitary). Thus T invariance, and hence the property of zero dipole moment, are observed only if f is pure imaginary, so that $T^{-1} H_1 T = H_1$.

The decay asymmetry depends on the imaginary part of f and is zero when f is real.

Conversely, for imaginary f the decay is distinctly asymmetric, but in the expression for the density of virtual particles the term with cos θ vanishes, the density distribution is spherically symmetric, and the dipole moment is zero.

We can consider a more general case, when, besides the interaction responsible for the transformations $N + \theta \rightleftarrows V$, there is an additional (say, Coulomb) potential between the particles N and θ. If the action of this potential on θ is taken into consideration, but it is assumed to be spherically symmetric, the conclusion of zero dipole moment for imaginary f remains in force: to the real term g in the equation corresponds a spherically symmetric real solution and to the imaginary term $i|f|$ cos θ corresponds an imaginary solution which is proportional to $|f|$ cos θ; no interference terms proportional to cos θ enter the expression for density, as before.

However, if f is real (so that the decay is perfectly symmetric when no additional potential is imposed), the next higher approximation reveals decay asymmetry: when $U(r)$ is introduced in the expression for the outgoing

wave, the phases of the s-wave and the p-wave change by different amounts α_s and α_p,* so that for the wave function ψ_a for $pr \gg 1$ we obtain the asymptotic expression

$$\psi_a = a' \exp(ikr + i\alpha_s)/r + ik\cos\theta \cdot b' \exp(ikr + i\alpha_p)/r \tag{56.13}$$

and for real f

$$j = \frac{k}{mr^2}[(a')^2 + k^2(b')^2 + 2a'b'\cos\theta\sin(\alpha_s - \alpha_p)]. \tag{56.14}$$

Here a' and b' are respectively proportional to g and f, and the proportionality coefficients are real. In the absence of a potential, the decay will nevertheless be asymmetric if the source is extended and g and f are real.

§ 57. ELECTRIC DIPOLE MOMENT OF AN UNSTABLE PARTICLE

In the previous section we found that in T-invariant theory a stable particle cannot have an electric dipole moment. This assertion, however, as was first shown in /209/, cannot be extended to unstable particles. Indeed, an unstable particle is characterized by an exponentially decaying state amplitude and is enveloped in an outgoing wave of emitted decay products. When time is reversed, the unstable particle does not simply change to an identical particle with opposite spin; it becomes something entirely new, a state with an exponentially growing amplitude surrounded by colliding decay products. Our proof of zero dipole moment thus clearly cannot be extended to cover unstable particles.

Bell /235/ maintains that unstable particles have no electric dipole moment either. In his treatment, however, he leans heavily on a peculiar definition of an unstable particle whose physical meaning is not immediately obvious.

Rigorous approach to this problem calls for a detailed study of the scattering of stable particles passing through an intermediate unstable state /210/. Consider a thought experiment in which the electric dipole moment of the unstable particle in the intermediate state precesses the spin of the stable scattered particles. We will show that no spin precession is observed in the stationary problem on account of its T-invariance. For the scattering of a wave packet, on the other hand, the spins are precessed, but in a very peculiar way, so that although the time-average spin precession is zero, it is different from zero at the initial instant.

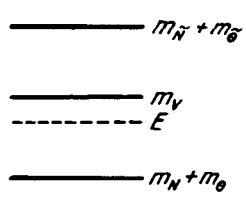

FIGURE 39.

For simplicity suppose that the unstable particle is neutral, and decays into neutral particles, which are not affected by the electric field. The model, however, should also contain charged particles responding to an electric

* α_s and α_p, which are functions of the potential $U(r)$, represent the increment of the phase of the regular solution of the homogeneous equation for s- and p-waves relative to the s- and p-waves of a free particle, $\psi_s = \sin kr/r$, $\psi_p = \cos\theta\left(\frac{\cos kr}{r} - \frac{\sin kr}{kr^2}\right)$.

field. A suitable model was proposed in /209/. This is a five-particle model, with $\theta, N, V, \tilde{N}$, and $\tilde{\theta}$. The particles θ and $\tilde{\theta}$ have spin 0; N, $\tilde{N}$, and V have spin 1/2; θ, N, and V are neutral, $\tilde{N}$ carries positive charge, and $\tilde{\theta}$ negative charge. The masses of the particles are so chosen that V may decay virtually into $\tilde{\theta}$ and $\tilde{N}$; the parity changes in this decay. Let further V decay actually into θ and $N (m_\theta + m_N < m_V < m_{\tilde{\theta}} + m_{\tilde{N}})$.

The term diagram of this system is shown in Figure 39, where the dashed line corresponds to the energy of N and θ. The system is immersed in an electric field of strength F pointing along the z axis. According to /210/, this system is described by the Hamiltonian.

$$\begin{aligned} H = {} & m_N \int N^+(r) N(r)\, dr + m_{\tilde{N}} \int \tilde{N}^+(r) \tilde{N}(r)\, dr + \\ & + m_\theta \int V^+(r) V(r)\, dr + \int \varphi_\theta^+(r) \left(\mu - \frac{\Delta}{2\mu}\right) \varphi_\theta(r)\, dr + \\ & + \int \varphi_{\tilde{\theta}}^+(r) \left(\tilde{\mu} - \frac{\Delta}{2\tilde{\mu}}\right) \varphi_{\tilde{\theta}}(r)\, dr + \left[f \int V^+(r) N(r) \varphi_\theta(r)\, dr + \right. \\ & \left. + g \int V^+(r) \tilde{N}(r) \varphi_{\tilde{\theta}}(r)\, dr + \text{h. c.} \right] + \\ & + ih \int V^+(r) \sigma \tilde{N}(r) \frac{d\varphi_{\tilde{\theta}}}{dr}\, dr + \text{h. c.} + \\ & + F \int \psi_{\tilde{N}}^*(r) z \psi_{\tilde{N}}(r)\, dr - F \int \psi_{\tilde{\theta}}^*(r) z \psi_{\tilde{\theta}}(r)\, dr. \end{aligned} \tag{57.1}$$

In T-invariant theory, $f^* = f$, $g^* = g$, $h^* = h$. The state vector is

$$\begin{aligned} \Phi = \Big[& \int \psi(r_1, r_2) N^+(r_1) \varphi_\theta^+(r_2)\, dr_1 dr_2 + \int \varphi(r_1) V^+(r_1)\, dr_1 + \\ & + \int \chi(r_1, r_2) \tilde{N}^+(r_1) \varphi_{\tilde{\theta}}^+(r_2) \Big] dr_1 dr_2 |0\rangle, \end{aligned} \tag{57.2}$$

and in the center-of-mass system the equations $H\Phi = E\Phi$ may be written as

$$E\psi = \left(m_N + \mu - \frac{\Delta}{2\mu}\right)\psi + f\delta(r)\varphi, \tag{57.3}$$

$$E\chi = \left(m_{\tilde{N}} + \tilde{\mu} - \frac{\Delta'}{2\tilde{\mu}}\right)\chi + Fz\chi + (g + ih\sigma\nabla)\delta(r)\varphi, \tag{57.4}$$

$$E\varphi = m_0\varphi + (g + ih\sigma\nabla)\chi(\rho) + f\psi(\rho), \tag{57.5}$$

where m_0 is the nonrenormalized mass of V, ρ is the cutoff radius, which goes to zero after renormalization.

To first approximation, we omit Fz. We obtain an exponential solution with complex energy $E_0 = \varepsilon - \frac{i\gamma}{2}$. The real and the imaginary parts of E_0 respectively determine the mass of the particle V and its decay probability. To simplify the expressions, we will assume the parity-nonconservation constant and the decay constant to be small, so that terms with f^4, h^2, etc., can be dropped. We moreover take $\gamma/2 \ll m_{\tilde{N}} + \tilde{\mu} - \varepsilon$, $\gamma/2 \ll \varepsilon - m_N - \mu$, which leads to the constraints

$$2\mu f^2 \ll \frac{\varkappa_0^2}{2\tilde{\mu} k_0}, \quad 2\mu f^2 \ll \frac{k_0^2}{2\mu k_0}.$$

Here and in what follows we use the notation

$$\varkappa^2 = 2\tilde{\mu}(m_{\tilde{N}} + \tilde{\mu} - E), \quad k^2 = 2\mu(E - m_N - \mu),$$
$$\varkappa_0^2 = 2\tilde{\mu}(m_{\tilde{N}} + \tilde{\mu} - \varepsilon), \quad k_0^2 = 2\mu(\varepsilon - m_N - \mu).$$

By (57.3)—(57.5) we get

$$m_0 = \varepsilon + \frac{\widetilde{\mu}g^2}{2\pi}\frac{1}{\rho} + \frac{\mu f^2}{2\pi}\frac{1}{\rho} - \frac{\widetilde{\mu}g^2}{2\pi}\varkappa_0, \tag{57.6}$$

$$\gamma = \frac{\mu f^2 k_0/\pi}{1 + \frac{\widetilde{\mu}g^2}{2\pi}\frac{\widetilde{\mu}}{\varkappa_0}}. \tag{57.7}$$

Note that if the second term in the denominator of (57.7) is much greater than 1, i.e., if the coupling between $\widetilde{N}, \widetilde{\theta}$, and V is sufficiently strong, we have

$$\gamma \approx 2\frac{\mu f^2}{\widetilde{\mu}g^2}\frac{k_0\varkappa_0}{\widetilde{\mu}}, \tag{57.8}$$

i.e., the decay probability of V markedly decreases. If now the particle V may decay into other particles $\widetilde{\widetilde{N}}$ and $\widetilde{\widetilde{\theta}}$, etc., additional positive terms will enter the denominator and the decay probability will diminish further. This effect in principle may be applied to explain the small width of some experimentally observed resonances.

We will now consider Fz to first order. Solving equations (57.3) and (57.4) for ψ and χ and inserting these functions in equation (57.5), we find that E_0 has no correction which is linear in F. The expression for δE_0 is thus the same as in the perturbation theory for complex E_0 /182, 183/, $\delta E_0 = F\int\tilde{\psi}_0^*\psi_0 z\,dr = 0$. The result $\delta E_0 = 0$ would appear at a first glance to contradict Newton's third law (action equals reaction). Indeed, the unstable particle produces a dipole electric field, since $\int\psi_0^*\psi_0 z\,dV \neq 0$, but the homogeneous electric field does not lead to a precession of its spin about the field vector, since no splitting is observed $\delta E_0 = 0$. This contradiction, however, is purely fictitious. It only means that unstable particles must not be manipulated like stable particles. If we remember that at the very beginning and at the end of the process we are dealing with stable particles (i.e., we do not dissociate the creation process from the decay process), no such paradox arises.

The precession effect may be observed for the scattering of θ by N. If before scattering, N is polarized along the z axis and the electric field is directed along the x axis, its polarization after scattering can be expected to precess through a certain angle α in the yz plane. For this effect to take place, it is further necessary that the state of the θ, N system have no definite energy, i.e., we must consider scattering of wave packets. (The effect of the electric dipole moment in scattering is a $[\sigma\sigma']F$ effect, and because of invariance under combined inversion it vanishes if the θN system has a definite energy.) Note that if the V particle has a magnetic moment and is immersed in a magnetic field, spin precession is observed in the stationary case also.

Our problem reduces to the solution of a system of equations

$$i\frac{d\psi}{dt} = \left(m_N + \mu - \frac{\Delta}{2\mu}\right)\psi + f\delta(r)\varphi, \tag{57.3'}$$

$$i\frac{d\chi}{dt} = \left(m_{\widetilde{N}} + \widetilde{\mu} - \frac{\Delta}{2\widetilde{\mu}}\right)\chi + Fz\chi + (g + ih\sigma\nabla)\delta(r)\varphi, \tag{57.4'}$$

$$i\frac{\partial\varphi}{\partial t} = m_0\varphi + (g + ih\sigma\nabla)\chi(\rho) + f\psi(\rho). \tag{57.5'}$$

We choose the following initial conditions:

$$\psi(r, 0) = \psi_0(r)\,\alpha,\ \chi(r, 0) = 0,\ \varphi(0) = 0;$$
$$\psi_0 = \frac{1}{2\sqrt{a\pi}\sqrt{\pi}} e^{-ipr - \frac{(r-r_0)^2}{2a^2}}; \tag{57.9}$$

α (β) corresponds to spin up (down). Let us calculate the derivative

$$\frac{ds(t)}{dt} = \frac{d}{dt}\left[\int \psi^* \frac{\sigma}{2}\,\psi\,dr + \int \chi^* \left(\frac{\sigma}{2} + [rp]\right)\chi\,dr + \varphi^* \frac{\sigma}{2}\varphi\right]. \tag{57.10}$$

Using (57.3')—(57.5'), we find

$$\frac{ds(t)}{dt} = \int \chi^*(r, t)\,[Fr]\,\chi(r, t)\,dr. \tag{57.11}$$

Integration of this equality over time from 0 to ∞ gives

$$\Delta s = \int \chi^*(r, t)\,[Fr]\,\chi(r, t)\,dr\,dt. \tag{57.12}$$

To evaluate Δs, we make use of the fact that the functions

$$\psi_k = \frac{1}{2\pi\sqrt{2}} \frac{-e^{-ikr} + S(k)e^{ikr}}{r}, \tag{57.13}$$
$$\chi_k = \frac{1}{2\pi\sqrt{2}} \frac{\tilde{\mu}}{\mu}(S(k) - 1)\frac{g + ih\sigma\nabla}{f}\frac{e^{-\varkappa r}}{r}, \tag{57.14}$$
$$\varphi_k = -\frac{S(k) - 1}{\sqrt{2}\mu f} \tag{57.15}$$

constitute a complete orthonormal system. Here

$$S(k) = \frac{(\varepsilon - E)\left[1 + \frac{\tilde{\mu}g^2}{2\pi}\frac{2\tilde{\mu}}{\varkappa + \varkappa_0}\right] + i\frac{\mu f^2 k}{2\pi}}{(\varepsilon - E)\left[1 + \frac{\tilde{\mu}g^2}{2\pi}\frac{2\tilde{\mu}}{\varkappa + \varkappa_0}\right] - i\frac{\mu f^2 k}{2\pi}} \tag{57.16}$$

(the formulas are written for $E < m_{\tilde{N}} + m_{\tilde{\theta}}$, for

$$E > m_{\tilde{N}} + m_{\tilde{\theta}},\ \varkappa \to -i\sqrt{2\tilde{\mu}(E - m_{\tilde{N}} - m_{\tilde{\theta}})}\,).$$

Expanding the functions $\psi_0, \psi, \chi, \varphi$ in this complete system and dropping exponentially small terms, we find that $\Delta s = 0$. Let us now find the first moment of spin precession, i.e., calculate the integral

$$\Delta s_1 = \int \frac{ds(t)}{dt}\,t\,dt. \tag{57.17}$$

Omitting the details, we give the final result:

$$\Delta s_1 = -\frac{F}{3}\frac{\tilde{\mu}^3}{\mu^2}\frac{gh}{f^2}\frac{1}{(2\varkappa)^3}\frac{\mu}{k}\,|S(k) - 1|^2. \tag{57.18}$$

On the other hand, given the exponential solution which describes the unstable particle, we readily find the electric dipole moment:

$$d = \int \psi_0^* z \psi_0 \, dr = \frac{gh}{4\pi} \frac{2}{3} \frac{\tilde{\mu}^3 \gamma}{\varkappa_0^3} \frac{1}{1 + \frac{\tilde{\mu} g^2}{2\pi} \frac{\tilde{\mu}}{\varkappa_0}}. \tag{57.19}$$

Using (57.7) we obtain

$$\Delta s_1 = -\tau (Fd\,\tau) \frac{\varkappa_0^3}{\varkappa^3} \frac{k_0}{k} \frac{1}{4} |S(k) - 1|^2, \tau = \frac{1}{\gamma}. \tag{57.20}$$

Expression (57.19) corresponds to the dipole moment of an exponentially decaying particle. The dipole moment is found to be proportional to γ, i.e., to the time derivative of the wave function. We can thus interpret (57.20) as follows: in the initial stages of scattering, when the amplitude of the wave function increases, the dipole moment has a certain sign and the spin precesses in a certain direction; toward the end of the scattering process, the amplitude of the unstable particle decreases, the dipole moment has a different sign, and the spin precesses in the opposite direction. On the average, the spin precession is thus zero. The moment of spin precession, as should have been expected, has the same sign as the precession angle of the decaying particles. The structure of the final expression is also clear: Δs_1 is proportional to the particle lifetime τ, the precession of the spin of the unstable particle (τFd), the resonance factor $\frac{1}{4}|S(k) - 1|^2$, which is equal to unity in resonance, and finally to a factor which does not vary much with energy and is also equal to unity in resonance.

We thus come to the following conclusion. If the polarization of the scattered particle is varied as a function of time during the scattering of a wave packet (time is reckoned from the formation of the wave packet), the polarization vector can be expected to precess first in one direction and then in another.

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